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Ph.D. Thesis

Mathematical analysis of Bose mixtures and related models: ground state theory and effective dynamics.

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Abstract

This PhD thesis contains new results on the mathematical study of Bose-Einstein condensation and the main part of it is devoted to mixtures of condensates, i.e., systems composed of multiple bosonic species in interaction.

We prove the validity of effective ground state theories for mixtures in the Gross-Pitaevskii and mean-field regime. We show that the ground state energy asymptotics, in the large-N limit, is captured by the minimum of a suitable one-body functional. Moreover, we prove that in the ground state all species exhibit Bose-Einstein condensation onto the minimizer of that functional.

For mixtures in the mean-field regime, we provide a rigorous justification of Bogoliubov's theory. This is done by computing the contribution to the ground state energy which is due to excited particles. We also prove a norm approximation for the ground state vector, in the Fock space norm.

From the time-dependent viewpoint, we prove for the first time the validity of the effective equations that were previously known due to heuristic physical arguments, and that are confirmed by robust experimental evidence. Our results show that, for mixtures in the Gross-Pitaevskii and mean-field regime, the effective dynamics is governed by a system of non-linear Schrödinger equations, one for each species of the mixture.

In the final part of the thesis we present additional results on problems and models related to the study on mixtures. We were able to derive the effective dynamics for spinor- and pseudo-spinor condensates. The equations that we obtain are precisely those of modern experiments with ultra-cold spin bosons. We also show that the mean-field model provide a time-dependent control of condensation that is very accurate for the typical duration times of experiments. A further result is the global well-posedness in the energy space of the singular Hartree equation. Last, we present new remarks on the adaptation of known techniques that one needs in order to prove the derivation of the magnetic Gross-Pitaevskii equation.

Contents

Introduction

This thesis contains the analysis of problems emerging from the mathematical study of Bose-Einstein condensation (BEC). The material is organized as follows.

- The present Introduction contains an overview on the effective ground state and dynamical description of BEC from the mathematical physics viewpoint, and a survey of the original results that will be discussed in detail through the thesis.

- Chapter 1 is devoted to the setup of the mathematical models for mixtures of condensates, the class of systems that represent the main object of this work.

- Chapters 2, 3, and 4 contain the main results on mixtures of condensates, based on my works [64], [67], [77]. First, we were able to compute the leading order in the number of particles of the ground state energy, and to prove BEC for the ground state, both in the mean-field and Gross-Pitaevskii regime. Furthermore, we were able to justify the validity of Bogoliubov theory for mixtures in the mean-field regime.
  In the time-dependent setting we proved persistence of condensation for mixtures in the mean-field and Gross-Pitaevskii regime, and hence the derivation of the system of non-linear Schrödinger equations describing the effective time evolution.

- Further results are presented in Chapter 5, based my works [66], [65], [68], [78]. These are the derivation of the effective dynamical equations for spinor and pseudo-spinor condensates, a quantitative estimate on the validity of the mean-field model, the proof of well-posedness of the singular Hartree equation, and a note on the derivation of the magnetic Gross-Pitaevskii equation.

Bose-Einstein condensation: a mathematical outlook

Bose-Einstein condensation is the physical quantum phenomenon, with no classical counterpart, which occurs in systems of identical bosons at very low temperatures when a macroscopic fraction of particles occupy the same one-body state. This was first conjectured theoretically by Bose [14] and Einstein [27] in the 1920's and then extensively studied through the following decades.

The theoretical investigation had no experimental counterpart until the mid 1990s, when cooling and trapping techniques were perfected enough to reproduce the conditions for condensation. In 1995, the teams of Cornell and Wieman at Boulder, and of Ketterle at MIT were for the first time able to observe BEC [6], [21]. This resulted in a Nobel prize in 2001, and in a continuously developing and very active mainstream in experimental physics.

The corresponding mathematical study of Bose-Einstein condensation has been an extraordinarily rich and active subject which dates back to the very first systematic treatment of Bogoliubov in the mid 1940's (that is, some 20 years after the theoretical discovery of BEC). In this Section we survey the mathematical formalism of BEC, introduce the concepts of effective ground state theory and effective dynamics, and discuss some important and by now classical result.

Mathematically, to a gas of N identical bosonic particles in three space dimensions and with no internal degrees of freedom, one associates the Hilbert space

$$\mathcal{H}_{N,\mathrm{sym}} \;:=\; L^2(\mathbb{R}^3)^{\otimes_{\mathrm{sym}} N}. \tag{0.1}$$

Elements of $\mathcal{H}_{N,\mathrm{sym}}$ are wave-functions $\psi_N(x_1,\dots,x_N)$ of N three-dimensional variables with full permutational symmetry among the variables, i.e. such that

$$\psi_N(x_1,\dots,x_N) \;=\; \psi_N(x_{\sigma(1)},\dots,x_{\sigma(N)})$$

for every permutation $\sigma\in\Sigma_N$, Σ_N being the group of permutations of N elements.

Let γ_N, a positive trace-class operator on $\mathcal{H}_{N,\mathrm{sym}}$ with unit trace, be the density matrix describing a state of a given bosonic system. Consistently with the physical notion of *occupation numbers*, the standard mathematical tool to express the occurrence of BEC when the system is in the state γ_N is the so-called *one-body marginal* (or one-body reduced density matrix)

$$\gamma_N^{(1)} \;:=\; \mathrm{Tr}_{N-1}\,\gamma_N\,. \tag{0.2}$$

Here the map $\mathrm{Tr}_{N-1}:\mathcal{B}_1(\mathcal{H}_{N,\mathrm{sym}})\to\mathcal{B}_1(L^2(\mathbb{R}^3))$ is the *partial trace* from trace class operators on $\mathcal{H}_{N,\mathrm{sym}}$ to trace class operators on $L^2(\mathbb{R}^3)$, defined by

$$\mathrm{Tr}_{L^2(\mathbb{R}^3)}(A\cdot\mathrm{Tr}_{N-1}T) \;:=\; \mathrm{Tr}_{\mathcal{H}_{N,\mathrm{sym}}}(A\otimes\mathbb{1}_{N-1}\cdot T),\qquad \forall A\in\mathcal{B}(L^2(\mathbb{R}^3)). \tag{0.3}$$

Thus, $\gamma_N^{(1)}$ is obtained by "tracing out" $N-1$ degrees of freedom from γ_N: for example, for a system in the pure state associated to the wave-function $\psi_N\in\mathcal{H}_{N,\mathrm{sym}}$, the corresponding one-body marginal $\gamma_N^{(1)}$ has kernel

$$\gamma_N^{(1)}(x,x') \;=\; \int_{\mathbb{R}^{3(N-1)}}\psi_N(x,x_2,\dots,x_N)\,\overline{\psi_N(x',x_2,\dots,x_N)}\,\mathrm{d}x_2\cdots\mathrm{d}x_N\,. \tag{0.4}$$

As a simple consequence of the above definition, the one-body marginal $\gamma_N^{(1)}$ has a complete set of real non-negative eigenvalues that sum up to 1, and being it the partial trace of a many-body state γ_N, it is natural to think of these eigenvalues as the occupation numbers in γ_N. This means that each eigenvalue of $\gamma_N^{(1)}$ is interpreted as the fraction of the N particles occupying the one-body state associated to the corresponding eigenvector.

In a sense to be specified in the given context, one says that the many-body state γ_N exhibits *condensation* with *condensate wave-function* $\varphi\in L^2(\mathbb{R}^3)$ ($\|\varphi\|=1$) if φ is an eigenvector of $\gamma_N^{(1)}$ that belongs to a non-degenerate eigenvalue that is by far larger than all other eigenvalues, i.e., it is almost 1 while all other eigenvalues are almost zero. In other words, $\gamma_N^{(1)}\approx|\varphi\rangle\langle\varphi|$, the rank-one projection onto φ. This notion of condensation becomes conceptually well-posed and mathematically rigorous in the limit $N\to\infty$ – a genuine thermodynamic limit, or some simpler prescription on $N\to\infty$ that mimics the thermodynamic limit. Notice that, strictly speaking, in order for a discussion on the $N \to \infty$ limit to make sense, one needs to specify a *sequence of systems* labeled by the number of particles and a sequence of states $\{\gamma_N\}_{N\in\mathbb{N}}$. This will be tacitly understood in every result we will present, and we will omit to mention it.

In particular, we shall consider the case of *complete* condensation, namely

$$\lim_{N\to\infty} \gamma_N^{(1)} \;=\; |\varphi\rangle\langle\varphi| \qquad \text{(complete BEC)}\,. \tag{0.5}$$

While the limit in (0.5) could be stated in several inequivalent operator topologies, simple considerations (see, e.g., [44, Section 2]) show that in this case weak operator convergence actually implies trace-norm convergence.

In (0.5) φ is customarily referred to as the *condensate wave-function* and in the presence of condensation the diagonal $\gamma_N^{(1)}(x,x)$ of the one-body marginal becomes, for large N, a good approximation of the condensate profile $|\varphi(x)|^2$. While the limit (0.5) is naturally interpreted as if the many-body state was almost completely factorized as $\varphi^{\otimes N}$, the closeness $\gamma_N^{(1)} \approx |\varphi\rangle\langle\varphi|$ is obviously much weaker than the actual closeness $\psi_N \approx \varphi^{\otimes N}$ in the norm of $\mathcal{H}_N$.

A number of mathematical problems naturally emerge from the definition (0.5), among which:

- the proof that Bose-Einstein condensation holds for physically relevant quantum states (e.g., ground states of interacting Hamiltonians, thermal states, ...),
- the computation of the energy of states exhibiting BEC,
- the proof that BEC is preserved as the system evolves in time according to many-body Schrödinger dynamics.

All the above problems have been studied extensively, particularly over the last two decades. The large majority of the results so far available lack of a rigorous control of the asymptotics (0.5) in a genuine thermodynamic limit. Instead, it is customary to investigate BEC in an ad hoc scaling limit in which the inter-particle interaction is N-dependent. Of course, the most relevant scalings are those that, even if differing from the thermodynamic limit, still mimic physically realistic situations.

We recall that the BEC property (0.5) amounts to having all particles in the same one-body orbital (at least as far as one-particle observables are concerned). It is of great interest to investigate whether the full many-body description boils down to a one-body *effective* model, depending on the condensate wave-function only, and not anymore on the full many-body state. This is of primary interest from the point of view of the problems listed above. For example, finding the exact N-body ground state energy or monitoring the N-body dynamics are computationally unreachable problems already for N exceeding a few units. It turns out that one can overcome such an obstruction by means of an *approximated* one-body model (which, of course, is computationally much more handy).

A physically relevant scenario in which it is possible to prove the validity of an effective model is the *Gross-Pitaevskii* (GP) regime. For a system of N bosons in three space dimensions, the many-body Gross-Pitaevskii Hamiltonian is the operator

$$H_N \;:=\; \sum_{j=1}^{N}\Big(-\Delta_{x_j} + U_{\mathrm{trap}}(x_j)\Big) + N^2 \sum_{j<k}^{N} V(N(x_j - x_k)) \tag{0.6}$$

acting on $\mathcal{H}_{N,\mathrm{sym}}$, with self-explanatory kinetic, trapping, and interaction terms.

We notice that a scaling prescription is present in the inter-particle interaction term, in the form of the replacement of the actual N-independent physical potential V with $N^2V(N\cdot)$. In such a regime the interaction among particles takes place on a spatial scale of order N^{-1}. Comparing the latter value with the mean inter-particle distance which, for bosons trapped in a box of order 1, is of order $N^{-1/3}$, shows that collisions are very rare, but with strong magnitude (because of the N^2 coupling constant). In this respect, (0.6) is a realistic model for *high dilution* and strong interaction.

It was a milestone result by Lieb, Seiringer, and Yngvason that there is an effective one-body theory describing low-energy properties of H_N. To formulate this precisely, let us introduce the Gross-Pitaevskii energy functional

$$\mathcal{E}[\varphi] \;:=\; \int_{\mathbb{R}^3} |\nabla\varphi(x)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^3} U_{\mathrm{trap}}(x)|\varphi(x)|^2 \,\mathrm{d}x + 4\pi a \int_{\mathbb{R}^3} |\varphi(x)|^4 \,\mathrm{d}x, \tag{0.7}$$

where $a \in \mathbb{R}$ is the scattering length of V (see Section 1.3 or [56, Appendix C] for a variational definition). The quartic term in $\mathcal{E}$ effectively represents the interaction between two particles described by the density $|\varphi(x)|^2$.

It was proven in [57], [56] by Lieb, Seiringer, and Yngvason that, for a regular enough U_{trap} with suitable confining properties, and for a non-negative, spherically symmetric V with finite scattering length and fast enough decay, the ground state energy per particle of H_N is asymptotically given by the minimum of the Gross-Pitaevskii functional, that is,

$$\lim_{N\to\infty} \frac{\min\sigma(H_N)}{N} \;=\; \min_{\substack{\varphi\in H^1(\mathbb{R}^3)\\ \|\varphi\|_{L^2}=1}} \mathcal{E}[\varphi] \tag{0.8}$$

(the assumptions on U_{trap} and V ensure both minima to be finite and attained).

Moreover, under the same assumptions, if φ_0 is the minimizer of $\mathcal{E}$, it was proven in [53], [56] by Lieb and Seiringer that the ground state ψ_N^{gs} of H_N exhibits condensation onto φ_0 in the sense (0.5), i.e.,

$$\lim_{N\to\infty} \gamma^{(1)}_{\psi_N^{\mathrm{gs}}} \;=\; |\varphi_0\rangle\langle\varphi_0|. \tag{0.9}$$

The results (0.8) and (0.9) were later generalized by Lieb and Seiringer [52] to rotating Bose gases and then obtained again by Nam, Rougerie, and Seiringer [74] with a different method that exploits the quantum de Finetti theorem. More recently, Boccato, Brennecke, Cenatiempo, and Schlein [12] were able to prove condensation with optimal convergence rate for a Bose gas in the GP regime and constrained in a unit torus.

A related investigation concerns the dynamical evolution of a system exhibiting BEC. Experimentally, a condensate is prepared by letting a trapped system 'cool down' to some low-energy state (say, the trap's ground state). Once this is attained, a perturbation of the system, typically a sudden change or switching-off of the confinement, lets the condensate evolve according to a non-trivial dynamics. It is a very robust experimental evidence that such an evolution preserves the condensate for a time scale long enough to be monitored, and that the profile of the condensate changes with time.

The phenomenon pictured above, i.e., *persistence of condensation*, has been well-known in physics for a long time, at least on a formal level. Its rigorous justification has been a major challenge in mathematical physics. It amounts to showing that the property (0.5) is preserved along the evolution $\gamma_N \mapsto \gamma_{N,t} = e^{-\mathrm{i}tH}\gamma_N e^{\mathrm{i}tH}$ governed by a given many-body Hamiltonian H, and hence to deriving rigorously the law $\varphi \mapsto \varphi_t$ that gives the condensate wave-function at later times. The many-body *linear* dynamics for $\gamma_{N,t}$ is then replaced by an effective *non-linear* dynamics for φ_t, the non-linearity being due to the inter-particle interaction and emerging in the form of a non-linear cubic self-interaction term in the Schrödinger equation for φ_t. This is completely analogous to the appearance of the quartic term in the Gross-Pitaevskii functional (0.7). In short (and for pure states), the dynamical problem consists of completing the following diagram, assuming that the first line holds at time $t = 0$:

$$\begin{tikzcd} \psi_N \arrow[r, "\text{partial trace}"] \arrow[d, "\substack{\text{many-body} \\ \textbf{linear}\text{ dynamics}}"'] & \gamma_N^{(1)} \arrow[r, "N\to\infty"] \arrow[d] & |\varphi\rangle\langle\varphi| \arrow[d, "\substack{\textbf{non-linear} \\ \text{Schrödinger eq.}}"] \\ \psi_{N,t} \arrow[r] & \gamma_{N,t}^{(1)} \arrow[r, "N\to\infty"] & |\varphi_t\rangle\langle\varphi_t| \end{tikzcd} \tag{0.10}$$

There is a vast literature on this class of investigations, covering different space dimensions ($d = 1, 2, 3$), a wide range of local singularities and long-distance decays for the inter-particle interactions, and various types of scaling limits in the many-body Hamiltonian.

An important result in this framework is the first rigorous derivation of the time-dependent Gross-Pitaevskii equation, due to Erdős, Schlein, and Yau [30], [28], [29], [31]. They considered a system governed by the Hamiltonian H_N defined in (0.6), having assumed $U_{\text{trap}} = 0$ and V to be non-negative, spherically symmetric, short range, bounded, with finite scattering length a. In such hypotheses, given an initial many-body wave-function ψ_N exhibiting condensation on $\varphi \in L^2(\mathbb{R}^3)$ and satisfying $\langle\psi_N, H_N\psi_N\rangle \leqslant CN$, they were able to prove that the evolved wave-function $\psi_{N,t} = e^{-\mathrm{i}tH_N}\psi_N$ exhibits condensation onto φ_t which solves the time-dependent Gross-Pitaevskii equation

$$\begin{cases} \mathrm{i}\partial_t\varphi_t \;=\; -\Delta\varphi_t + 8\pi a|\varphi_t|^2\varphi_t \\ \varphi_t|_{t=0} \;=\; \varphi. \end{cases} \tag{0.11}$$

Their proof, based on the hierarchical structure of the evolution equations for all the partial marginals (the BBGKY hierarchy) and equivalent to the Schrödinger equation, did not provide a quantitative rate for the convergence towards $|\varphi_t\rangle\langle\varphi_t|$, because the limit was controlled by compactness. The convergence rate was later obtained by Pickl [82], by Benedikter, de Oliveira, and Schlein [8], and by Brennecke and Schlein [15] through different methods.

For a comprehensive outlook on the derivation of effective equations from quantum systems, we refer to the review [9] and references therein. We remark that the problem has involved a variety of approaches and techniques from analysis to operator theory, kinetic theory, and probability.

It is also worth remarking that the scaling defined by (0.6) is not the only one considered in the literature. Another relevant prescription amounts to rescaling the coupling constant only, by a factor N^{-1}, hence considering an interaction term

$$\frac{1}{N}\sum_{j<k}^{N} V(x_j - x_k).$$

This is called *mean-field* regime and, effectively as $N \to \infty$, it describes a gas of particle that are weakly coupled and interact on a range of the same order as the size of the region in which they are trapped. The effective energy functional describing the low energy properties of a mean-field Hamiltonian is the *Hartree* functional

$$\widetilde{\mathcal{E}}[\varphi] \;:=\; \int_{\mathbb{R}^3} |\nabla\varphi|^2\,\mathrm{d}x + \int_{\mathbb{R}^3} U_{\text{trap}}(x)|\varphi(x)|^2\,\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^3} \big(V * |\varphi|^2\big)(x)|\varphi(x)|^2,$$

while the effective evolution equation that completes the diagram (0.10) is the Hartree equation

$$\mathrm{i}\partial_t\varphi_t \;=\; -\Delta\varphi_t + U_{\mathrm{trap}}\,\varphi_t + (V * |\varphi_t|^2)\varphi_t. \tag{0.12}$$

The mean-field regime has been extensively studied in the past decades. Despite being a first approximation, we will show in Section 5.1 that the mean-field effective dynamics still allows one to control the occurrence of condensation with high precision *for the whole typical duration of modern experiments* (see also [65]).

To conclude this Section, we mention that a further non-trivial result proven in particular scaling regimes is the validity of the *Bogoliubov's theory*. This allows one to monitor the role of the fraction of particles that are not in the condensate (often called *excitations*), hence providing non-trivial next-to-leading information on the ground state energy and ground state asymptotics.

The first proofs of Bogoliubov's theory, due to Seiringer [88] for particles in a homogeneous box, Grech and Seiringer [35] for particles in a trapping potential, and Lewin, Nam, Serfaty, and Solovej [49] for more general many-body systems, were valid in the mean-field regime. Only more recently Boccato, Brennecke, Cenatiempo, and Schlein [11] were able to justify Bogoliubov's theory in the Gross-Pitaevskii regime for a Bose gas in a homogeneous box.

For an extended discussion on features and roles of mean-field, Gross-Pitaevskii, and other regimes, we refer to [63].

Main results of the thesis

The main results presented in this thesis concern the *effective ground state and dynamical description of condensate mixtures.*

A large amount of theoretical and experimental studies on Bose gases involve the interaction among two or more atomic species, each of which is in a condensed state (see, e.g., [84, Section 12.11] and references therein). These configurations are typically realized using heteronuclear mixtures of ^{41}K-^{87}Rb [70], ^{41}K-^{85}Rb [71], ^{39}K-^{85}Rb [61], ^{85}Rb-^{87}Rb [80]. The two species are called *components* and the whole system is a *multi-component condensate*, or also *mixture of condensates*, or *condensate mixture.*

Physical arguments corroborated by experimental data show that the effective non-linear description works to a very good degree of approximation, and depends on as many orbitals as the number of components of the mixture. For example, the ground state energy of a m-component mixture is obtained by minimizing a functional on a m-particle Hilbert space. Analogously, the effective dynamics of a m-fold mixture is described by a system of m coupled non-linear Schrödinger equations, the coupling among them accounting how each of the m components affect the evolution of the others.

Although these facts are by now well-known in the physics literature, no complete mathematical treatment of mixtures of Bose gases was available at the time the present work started.

We shall consider a large three-dimensional system consisting of two distinguishable populations of identical bosons, with two-body interactions among particles of the same species and of different species (the extension to an arbitrary number m of different species is trivial and hence omitted). We also allow for the possibility of external fields trapping the particles. The precise definitions of the models and of the scaling limits, together with the mathematical tools needed to properly treat the problem, will be the main content of Chapter 1.

Acting on the Hilbert space

$$\mathcal{H}_{N_1,N_2,\mathrm{sym}} \;:=\; L^2_{\mathrm{sym}}(\mathbb{R}^{3N_1}) \otimes L^2_{\mathrm{sym}}(\mathbb{R}^{3N_2})$$

of two different bosonic species of, respectively, N_1 and N_2 identical particles, we will then consider two self-adjoint Hamiltonians $H^{\mathrm{GP}}_{N_1,N_2}$ and $H^{\mathrm{MF}}_{N_1,N_2}$ (for the Gross-Pitaevskii and mean-field regimes) whose explicit definition will be given by (1.13) and (1.14) in Chapter 1.

As will be discussed in Section 1.2, the appropriate language to formulate condensation for mixtures and to monitor the effective dynamics is the one of generalized reduced density matrices for Bose gases with two distinguishable components. The key object is the $(1,1)$-particle reduced marginal, which, for a system described by the wave-function $\psi_{N_1,N_2} \in \mathcal{H}_{N_1,N_2,\mathrm{sym}}$, is defined by

$$\gamma^{(1,1)}_{\psi_{N_1,N_2}} \;=\; \mathrm{Tr}_{N_1-1} \otimes \mathrm{Tr}_{N_2-1} \, |\psi_{N_1,N_2}\rangle\langle\psi_{N_1,N_2}|, \tag{0.13}$$

hence tracing out all degrees of freedom except for those of one particle for each species.

In analogy with (0.5), we say that a state with wave-function $\psi_{N_1,N_2} \in \mathcal{H}_{N_1,N_2,\mathrm{sym}}$ exhibits *double-component Bose-Einstein condensation* if there exist two *condensate wave-functions* $u, v \in L^2(\mathbb{R}^3)$ such that

$$\lim_{N_1,N_2\to\infty} \gamma^{(1,1)}_{\psi_{N_1,N_2}} \;=\; |u\otimes v\rangle\langle u \otimes v|. \tag{0.14}$$

This definition was formulated in my work [67]. As presented in Section 1.2, (0.14) has a clear interpretation in terms of *occupation numbers*. We shall also discuss in Chapter 1 the joint limit $N_1, N_2 \to \infty$, and the topologies in which it holds.

In the remaining part of this Section we informally present the main results we obtained, which are the contents of Chapters 2, 3, and 4. We also briefly discuss the techniques we used in the proofs. As will be thoroughly pointed out, our results generalize the one-component analysis of BEC presented in the previous Section. We found that several among the many alternative techniques developed so far to investigate one-component problems can be adapted to the multi-component setting, with an amount of non-trivial modifications that depend on the considered techniques.

Ground state properties in the Gross-Pitaevskii regime

Chapter 2 presents the ground state theory for BEC mixtures in the Gross-Pitaevskii regime. In analogy with (0.8) and (0.9), we control the energy asymptotics and prove condensation for the ground state.

For the ground state energy $\inf\sigma(H^{\mathrm{GP}}_{N_1,N_2})$ and the minimum e_{GP} of the two-component GP functional defined in (1.18), we prove in Theorem 2.1 (*ii*) that

$$\lim_{N_1,N_2\to\infty} \frac{\inf\sigma(H^{\mathrm{GP}}_{N_1,N_2})}{N_1+N_2} \;=\; e_{\mathrm{GP}}. \tag{0.15}$$

Moreover, in Theorem 2.1 (*iii*), we prove that the ground state ψ_{N_1,N_2} of $H^{\mathrm{GP}}_{N_1,N_2}$ exhibits condensation on the *unique* minimizer (u_0, v_0) of the GP functional, i.e.,

$$\lim_{N_1,N_2\to\infty} \gamma^{(1,1)}_{\psi_{N_1,N_2}} \;=\; |u_0\otimes v_0\rangle\langle u_0 \otimes v_0|. \tag{0.16}$$

These results are based on my work [64].

To prove such results we adapted a technique by Nam, Rougerie, and Seiringer [74], based on the quantum de Finetti theorem [92], [41], [4], [47], by introducing suitable modifications that take into account the two-component nature of the system. The upper bound for energy convergence is proven by producing a trial function with the correct amount of correlations between particles. The lower bound is proven using Dyson Lemma, a result that allows one to replace an interaction potential that scales very singularly in N with a less singular one (in the same spirit as in [57], [55], [52], [74]). A crucial ingredient through all the proof is the quantum de Finetti theorem, that rigidly fixes the structure of limits of reduced density matrices. In Section 1.4 we will state and prove the quantum de Finetti theorem for a system consisting of two bosonic species.

We are also able to rigorously justify for the first time in the context of effective theories the 'miscibility' condition between the two species. It is experimentally known (see, e.g., [32], [60, Section 15.2], [36, Section 16.2.1] and [84, Section 21.1]) that, if a_1, a_2 are the scattering lengths of the infra-species interactions and a_{12} is the scattering length of the inter-species interaction, then

$$a_1 a_2 \;\geqslant\; a_{12}^2 \tag{0.17}$$

implies absence of *phase separation* in the ground state: the two species can condense on spatially overlapping orbitals. In our Theorem 2.1, thanks to (0.17) we are able to directly prove uniqueness of the minimizer of the GP functional.

Ground state properties in the mean-field regime

Chapter 3 presents the analysis of ground state properties in the mean-field regime, based on my work [64]. We are able for the first time to prove the validity of Bogoliubov theory for mixed Bose gases, hence providing additional results with respect to the Gross-Pitaevskii case.

As a first step, we prove that the ground state energy per particle of $H^{\mathrm{MF}}_{N_1,N_2}$ converges towards the minimum e_{H} of the Hartree functional (1.17), i.e., (see Theorem 3.2 (II))

$$\lim_{N_1,N_2\to\infty} \frac{\inf\sigma(H^{\mathrm{GP}}_{N_1,N_2})}{N_1+N_2} \;=\; e_{\mathrm{H}}, \tag{0.18}$$

and that the ground state $\psi^{\mathrm{gs}}_{N_1,N_2}$ exhibits BEC on the minimizer (u_0, v_0) of the Hartree functional, i.e., (see Theorem 3.2 (III))

$$\lim_{N_1,N_2\to\infty} \gamma^{(1,1)}_{\psi^{\mathrm{gs}}_{N_1,N_2}} \;=\; |u_0\otimes v_0\rangle\langle u_0\otimes v_0|. \tag{0.19}$$

These results are the direct counterpart of those obtained in the GP regime. In addition to that, we are able to prove that the next contribution to the many-body ground state energy comes from the ground state energy of the *Bogoliubov Hamiltonian* $\mathbb{H}$. Hence, we obtain an expansion in powers of N_1, N_2 which reads (see Theorem 3.1 (iii))

$$\inf\sigma(H^{\mathrm{MF}}_{N_1,N_2}) \;=\; (N_1+N_2)e_{\mathrm{H}} + \inf\sigma(\mathbb{H}) + o(1), \qquad \text{as } N\to\infty. \tag{0.20}$$

The operator $\mathbb{H}$, quadratic in creators and annihilators, describes the energy of particles excited outside of the condensate (that is, orthogonal to the minimizer of the Hartree functional). It is explicitly characterized as a second quantized form of the Hessian of the Hartree functional evaluated at the minimizer.

Furthermore, in Theorem 3.1 (*iv*), we prove that the ground state Φ^{gs} of $\mathbb{H}$ provides a norm approximation to the many-body ground state in the sense that

$$\lim_{N_1,N_2\to\infty} U_{N_1,N_2}\psi^{\mathrm{gs}}_{N_1,N_2} = \Phi^{\mathrm{gs}} \tag{0.21}$$

in the Fock space norm topology, for a unitary operator U_{N_1,N_2} that will be defined and discussed in Section 3.4.

The proof of Theorem 3.1 is based on a very general method to justify Bogoliubov theory introduced in [49] by Lewin, Nam, Serfaty, and Solovej, which we adapted to the two-component setting. A key point for its applicability is the possibility of localizing a state in the Fock space on sectors with at most M particles, with $M \leqslant N$. This is allowed by Proposition 3.13, a consequence of the IMS formula already proven in [50, Theorem A.1] and [49, Proposition 6.1]. We are then able to prove that an appropriate choice of M in terms of N allows to obtain the energy and ground state asymptotics.

Effective dynamics of condensate mixtures

Our next concern, in analogy with the one-component analysis, is the problem of persistence in time of condensation for mixtures. We were able to prove that, both in the Gross-Pitaevskii and mean-field regime, double-component condensation is preserved by many-body time evolution, and the effective dynamics is ruled by a system of coupled non-linear Schrödinger equations. These results are presented in Chapter 4, based on my works [67], [77].

The effective equations that we derive are precisely those that physical heuristics produce (see, e.g., [84, Chapter 21]), in extraordinary agreement with experimental data.

As a matter of fact, our results started an investigation on the effective dynamics of condensate mixtures that has attracted interest and further contributions. Subsequent result are due to Anapolitanos, Hott, and Hundertmark [5], who treated more singular interactions, and to de Oliveira and Michelangeli [22], who monitored the fluctuations around the dynamics of coherent states in Fock space.

We consider a two species Bose gas prepared at time $t = 0$ with a wave-function ψ_{N_1,N_2} that exhibits condensation onto $u, v \in L^2(\mathbb{R}^3)$. We are then able to prove that the evolved state $\psi_{N_1,N_2,t} = e^{-\mathrm{i}tH^{\mathrm{MF}}_{N_1,N_2}}\psi_{N_1,N_2}$ exhibits condensation for all $t \in \mathbb{R}$, i.e.,

$$\lim_{N_1,N_2\to\infty} \gamma^{(1,1)}_{\psi_{N_1,N_2,t}} \;=\; |u_t \otimes v_t\rangle\langle u_t \otimes v_t|, \tag{0.22}$$

where (u_t, v_t) solves the effective system (4.3).

We prove an analogous result for the Gross-Pitaevskii regime as well, with the evolution of (u_t, v_t) governed now by (4.19). Here, however, the nature of the technique requires to assume, for the initial datum, the following energy compatibility between many-body theory and effective theory

$$\lim_{N_1,N_2\to\infty} \frac{\langle \psi_{N_1,N_2}, H^{\mathrm{GP}}_{N_1,N_2}\psi_{N_1,N_2}\rangle}{N_1+N_2} \;=\; \mathcal{E}^{\mathrm{GP}}[u,v]. \tag{0.23}$$

Here $\mathcal{E}^{\mathrm{GP}}$ is the two-component Gross-Pitaevskii functional (1.18).

We employ a robust method, invented and refined in a recent series of papers by Pickl [83], [81], [82], in collaboration with Knowles [44]. This technique monitors how the displacement between full theory and effective theory changes with time by means of an ad hoc ‘counting’ of the amount of particles in the many-body state that occupy the $(1,1)$-body state $u_t \otimes v_t$. This counting is implemented by the functional

$$\alpha^{(1,1)}_{\psi_{N_1,N_2,t}} \;=\; 1 - \langle u_t \otimes v_t, \gamma^{(1,1)}_{\psi_{N_1,N_2,t}} u_t \otimes v_t \rangle, \tag{0.24}$$

which measures how much the expectation of the $(1,1)$-marginal on the condensate wave-function differs from its maximal value 1.

Analogously to the one-component case, we prove that in the limit $N_1, N_2 \to \infty$ the vanishing of the α-functional is equivalent to condensation, and, by assumption, this is the case for our initial datum. The technique then goes through a Grönwall argument that propagates the smallness of $\alpha^{(1,1)}_{\psi_{N_1,N_2,t}}$ for all $t > 0$.

Further related results

The final part of this thesis contains the analysis of a number of problems and models related to the study on mixtures of Bose gases. This has produced additional results that cannot be comprehensively described within the remaining space and therefore are only surveyed in Chapter 5. Let us briefly present the material in this Section.

Effective dynamics of pseudo-spinor and spinor condensates

Mixtures of BEC constitute the first object of a more general research programme, pursued in the course of this thesis’ work, focused on ‘composite’ condensates, i.e., Bose systems whose condensation is not described by a single scalar orbital. This broad expression includes not only mixtures of different atomic species, which are the main object of this thesis, but also systems in which bosons of the same species populate different hyperfine states [72], [62], [37], [38].

The first experimental breakthroughs were found with magnetically-trapped gases of ^{87}Rb that turned out to be quite long-lived due to the fortunate circumstance that the singlet and triplet scattering lengths have almost the same value, which greatly suppresses the spin-spin collision rate. This allows for the creation of Bose-Einstein condensates where a macroscopic occupation of particles can be driven coherently through two hyperfine levels, typically the $|F = 1, m_F = -1\rangle$, the $|F = 2, m_F = 2\rangle$, or the $|F = 2, m_F = 1\rangle$ states. Such systems are referred to as *pseudo-spinor condensates*: only a restricted number of hyperfine levels contribute effectively to the experiment, through the coupling with a resonant external magnetic field (Rabi coupling).

In contrast, a highly off-resonant magnetic confinement can trap the atoms irrespectively of their hyperfine state: in this case the spin becomes a new degree of freedom and this produces interacting Bose gases of ultra-cold atoms where the spatial two-body interaction is mediated by a spin-spin coupling. When such systems exhibit a macroscopic occupation of the same one-body state, the order parameter being now a vector in the hyperfine spin space, one speaks of *spinor condensates*.

Section 5.1 contains results on the effective dynamics of pseudo-spinor and spinor condensates, based on my works [66], [65]. The main statements are Theorem 5.1 and Theorem 5.2, and show that in both cases the effective dynamics is ruled by suitable systems of non-linear Schrödinger equations.

The equations we derive are precisely those predicted by physical arguments, and they agree with experimental data (see, e.g., [19] for a modern realization of a spinor condensate of spin-1 bosons).

Our proofs are the first adaptations of Pickl's counting method to bosonic systems with internal degrees of freedom. We were able to control the new contribution coming from a (time-dependent) external magnetic field that causes transfer of norm between the different spin levels.

In Section 5.2 we present a quantitative analysis, based on recent experimental data, of the fidelity of the mean-field model (in fact valid also for single- and multi-component BEC and pseudo-spinors). Despite the character of 'first approximation only', we show that it yields a control of the time-dependent indicator of condensation that remains very small *for all the typical duration of an experiment on the dynamics of spinor condensates.*

Well-posedness of the singular Hartree equation

The singular Hartree equation is a version of the Hartree equation in which the ordinary Laplace operator is replaced by its singular perturbation (described, e.g., in [3, Chap. I.1] and [69]). It is believed to describe the effective dynamics of Bose-Einstein condensates in which every particle experiences a very peaked and localized singularity. A rigorous proof of this fact is at the moment lacking. Yet, since a fundamental prerequisite of *all* known derivation techniques is the (at least local) well-posedness of the effective equation, we aimed at establishing such first ingredient.

The content of Section 5.3 is the global well-posedness in the energy space of the singular Hartree equation. This is based on my work [68]. We are able to prove local well-posedness for various regimes of regularity, and then use conservation laws to prove global well-posedness in the mass and energy space.

Our proof relies on the recent results [23], [33] (by my collaborators together with Dell'Antonio, Georgiev and Yajima) which provide full characterization of the perturbed Sobolev spaces, namely the form domains of fractional powers of the perturbed Laplacian.

Derivation of the Gross-Pitaevskii equation with magnetic Laplacian

Section 5.4 contains a discussion of the derivation of the Gross-Pitaevskii equation with the magnetic Laplacian. Even though this result was already claimed in [82], the adaptations of the known Pickl's counting technique to the magnetic case are non-trivial in various aspect, and were not present in literature. This gap was eventually closed in my work [78], whose main result is reported in Section 5.4. The proof makes direct reference to the work [82], with a step-by-step description of the needed modifications.

Chapter 1

Mathematical description of condensate mixtures

This Chapter presents the mathematical tools and results needed for the study of mixtures of Bose-Einstein condensates. While part of the discussion is based on standard quantum mechanics, some results are based on my works [67] (in collaboration with Michelangeli) and [64] (in collaboration with Michelangeli and Nam).

1.1 Hilbert space and reduced density matrices

The following Hilbert space will be considered

$$\mathcal{H}_{N_1,N_2,\mathrm{sym}} := L^2_{\mathrm{sym}}(\mathbb{R}^{3N_1}, \mathrm{d}x_1, \dots, \mathrm{d}x_{N_1}) \otimes L^2_{\mathrm{sym}}(\mathbb{R}^{3N_2}, \mathrm{d}y_1, \dots, \mathrm{d}y_{N_2}) . \tag{1.1}$$

It is naturally associated to a system consisting of two different families of, respectively, N_1 and N_2 identical bosons. An element ψ_{N_1,N_2} of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ is a square-integrable wave-function with two distinct sets of variables such that

$$\psi_{N_1,N_2}(x_1, \dots, x_{N_1}; y_1, \dots, y_{N_2})$$

is invariant under exchange of any two x-variables or any two y-variables, with no overall permutation symmetry among the two sets of variables.

Most of the statements presented in this work are proven in suitable limits of infinitely many particles. As already mentioned in the Introduction, in principle this would require for a *sequence* of systems labeled by N_1 and N_2 to be considered. We shall always consider systems labeled by fixed, but generic, N_1 and N_2, in this way implicitly defining a whole sequence.

We will only consider the case in which, as $N_1, N_2 \to +\infty$, there exist $c_1, c_2 \in (0,1)$ such that

$$c_j = \lim_{N_1,N_2 \to +\infty} \frac{N_j}{N}, \quad \text{for } j \in \{1,2\}, \qquad \text{where } N := N_1 + N_2. \tag{1.2}$$

This is a realistic requirement, since it merely asks that none of the two species is overwhelmingly populated with respect to the other, and the two populations remain comparable. It is not restrictive to assume that the ratios N_1/N and N_2/N are fixed and equal to, respectively, c_1 and c_2, and so shall we henceforth. Such choice implies that, given c_1, c_2, the numbers N_1, N_2, and N are specified once one of the three is known, say N. For this reason, we will often indicate with the subscript N quantities that actually depend on N_1 and N_2, and omit to keep track of the dependence on c_1 and c_2, which are assumed to be fixed once and for all.

States on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ are density matrices, that is, positive trace-class operators with unit trace, with a bosonic symmetry naturally inherited from the Hilbert space. As a concrete example, one might think of a factorized density matrix $\gamma_{N_1}\otimes\gamma_{N_2}$ where, for $j=1,2$, γ_{N_j} is a density matrix on $L^2_{\mathrm{sym}}(\mathbb{R}^{3N_j})$. A generic state of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, however, need not be factorized.

Pure states on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ are rank one projections, and, up to a phase, they are in one-to-one correspondence with unit vectors (wave-functions) in $\mathcal{H}_{N_1,N_1,\mathrm{sym}}$. We will indifferently use the notations γ_{ψ_N} and $|\psi_N\rangle\langle\psi_N|$ to indicate the pure state associated to $\psi_N\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$.

The density matrix (or, in the case of pure states, the wave-function) contains the complete information on the state of the system. Given an observable $\mathcal{O}$, i.e., a bounded self-adjoint operator on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, its expectation on a state γ is given by

$$\langle\mathcal{O}\rangle_\gamma \;:=\; \mathrm{Tr}\,\gamma\,\mathcal{O}.$$

The phenomenon we shall investigate is Bose-Einstein condensation for mixtures, which is efficiently monitored in terms of observables that depend on few particles of the system. Hence, when condensation occurs, complete knowledge of the full density matrix is often not needed, being it enough to have information on the *two-component reduced density matrices*.

Given a pure state with wave-function $\psi_N\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, for any couple of integers k_1,k_2 such that $k_1\leqslant N_1$ and $k_2\leqslant N_2$, the (k_1,k_2)-particles reduced density matrix associated to ψ_N is defined by

$$\gamma^{(k_1,k_2)}_{\psi_N} \;:=\; \mathrm{Tr}_{N_1-k_1}\otimes\mathrm{Tr}_{N_2-k_2}\,|\psi_N\rangle\langle\psi_N|. \tag{1.3}$$

The operation in (1.3) amounts to tracing out N_1-k_1 degrees of freedom in the first component and N_2-k_2 in the second. It is straightforward to see that $\gamma^{(k_1,k_2)}_{\psi_N}$ is a positive trace-class operator with unit trace which, for $k_1,k_2\geqslant 1$, acts on $L^2_{\mathrm{sym}}(\mathbb{R}^{3k_1})\otimes L^2_{\mathrm{sym}}(\mathbb{R}^{3k_2})$. Its integral kernel reads

$$\begin{aligned}
&\gamma^{(k_1,k_2)}_{\psi_N}(x_1,\dots,x_{k_1},x'_1,\dots,x'_{k_1};y_1,\dots,y_{k_2},y'_1,\dots,y'_{k_2}) \;=\\
&=\int_{\mathbb{R}^{3(N_1-k_1)}}\int_{\mathbb{R}^{3(N_2-k_2)}}\mathrm{d}x_{k_1+1}\cdots\mathrm{d}x_{N_1}\mathrm{d}y_{k_2+1}\cdots\mathrm{d}y_{N_2}\\
&\quad\times\psi_N(x_1,\dots,x_{k_1},x_{k_1+1},\dots,x_{N_1};y_1,\dots,y_{k_2},y_{k_2+1},\dots,y_{N_2})\\
&\quad\times\overline{\psi_N}(x'_1,\dots,x'_{k_1},x_{k_1+1},\dots,x_{N_1};y'_1,\dots,y'_{k_2},y_{k_2+1},\dots,y_{N_2})\,.
\end{aligned} \tag{1.4}$$

In the extremal cases, (1.3)-(1.4) above define reduced density matrices $\gamma^{(k_1,0)}_{N_1,N_2}$ and $\gamma^{(0,k_2)}_{N_1,N_2}$ acting, respectively, on the single-species bosonic spaces $L^2_{\mathrm{sym}}(\mathbb{R}^{3k_1})$ and $L^2_{\mathrm{sym}}(\mathbb{R}^{3k_2})$, that is, all the degrees of freedom of one of the two components are traced out.

1.2 Double-component BEC and indicators of condensation

A particularly important reduced density matrix associated to a wave-function $\psi_N\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ is the operator $\gamma^{(1,1)}_{\psi_N}$. Being it, as an immediate consequence of (1.3), a positive trace class operator on $L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)$ with unit trace, it can be written as

$$\gamma^{(1,1)}_{\psi_N} \;=\; \sum_j \lambda_j|z_j\rangle\langle z_j|, \tag{1.5}$$

where $\{z_j\}_j$ is an orthonormal (not necessarily complete) family of vectors in $L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)$. The positive reals $\{\lambda_j\}_j$ sum up to one and are interpreted as occupation numbers, because λ_j represents the probability that, in the many-body state γ_{ψ_N}, one particle of the first species *and* one of the second species are jointly described by the orbital z_j.

In analogy with the single-component case, complete Bose-Einstein condensation in two components occurs when only one occupation number is macroscopically different from zero, while all the others are negligible. This should be meant in a suitable limit, and is tantamount as to say that the operator $\gamma_{\psi_N}^{(1,1)}$ converges to a rank one projection on $L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)$. Hence, we say that a pure state γ_{ψ_N} associated to $\psi_N\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ exhibits asymptotic 100% Bose-Einstein condensation in two components with *condensate wave-functions* u and v if

$$\lim_{N_1,N_2\to\infty}\gamma_{\psi_N}^{(1,1)}=|u\otimes v\rangle\langle u\otimes v|,\tag{1.6}$$

where $u,v\in L^2(\mathbb{R}^3)$ with $\|u\|=\|v\|=1$. Even if a priori the limit in (1.6) could be stated in several inequivalent operator topologies, from the trace norm to the weak operator topology, the bounds

$$\begin{aligned}1-\big\langle u\otimes v,\gamma_{\psi_N}^{(1,1)}u\otimes v\big\rangle_{L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)}\;&\leqslant\;\mathrm{Tr}\,\big|\gamma_{\psi_N}^{(1,1)}-|u\otimes v\rangle\langle u\otimes v|\big|\\&\leqslant\;2\sqrt{1-\big\langle u\otimes v,\gamma_{\psi_N}^{(1,1)}u\otimes v\big\rangle_{L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)}}\end{aligned}$$

(see Lemma 1.2 below) show that the occurrence of the convergence $\gamma_{\psi_N}^{(1,1)}\to|u\otimes v\rangle\langle u\otimes v|$ is equivalently monitored in any of them.

The limit in (1.6) expresses, in the interpretation of occupation numbers, the idea that the actual many-body state has the double-condensate form $u^{\otimes N_1}\otimes v^{\otimes N_2}$, although the vanishing of $\gamma_{\psi_N}^{(1,1)}-|u\otimes v\rangle\langle u\otimes v|$ is *much weaker* than the actual vanishing of $\|\psi_N-u^{\otimes N_1}\otimes v^{\otimes N_2}\|_{\mathcal{H}_{N_1,N_2,\mathrm{sym}}}$.

Observe that the distinguishability of the two species results in a precise ordering in the product $u\otimes v\in L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)$ of the two condensate functions. Thus, even in the case $u=v$, the double condensation $\gamma_{\psi_N}^{(1,1)}\approx|u\otimes u\rangle\langle u\otimes u|$ expresses the fact that each component undergoes BEC with *the same spatial profile* of the condensate: the two condensates then sit on top of each other, while the two species remain distinguishable.

In order to prove a limit of type (1.6) to hold, it is customary to introduce appropriate indicators of convergence. Given a wave-function $\psi_N\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, two one-body orbitals $u,v\in L^2(\mathbb{R}^3)$ with $\|u\|=\|v\|=1$, and two integers k_1,k_2 with $k_j\leqslant N_j$, $j=1,2$, define

$$\alpha_{\psi_N}^{(k_1,k_2)}\;:=\;1-\big\langle u^{\otimes k_1}\otimes v^{\otimes k_1}\,,\,\gamma_{\psi_N}^{(k_1,k_2)}\,u^{\otimes k_1}\otimes v^{\otimes k_2}\big\rangle_{\mathcal{H}_{k_1,k_2,\mathrm{sym}}}\tag{1.7}$$

and

$$R_{\psi_N}^{(k_1,k_2)}\;:=\;\mathrm{Tr}\,\big|\,\gamma_{\psi_N}^{(k_1,k_1)}-|u^{\otimes k_1}\otimes v^{\otimes k_2}\rangle\langle u^{\otimes k_1}\otimes v^{\otimes k_2}|\,\big|\,.\tag{1.8}$$

Both quantities measure a displacement of the marginal $\gamma_{\psi_N}^{(k_1,k_1)}$ from $|u^{\otimes k_1}\otimes v^{\otimes k_2}\rangle\langle u^{\otimes k_1}\otimes v^{\otimes k_2}|$, which is the (k_1,k_2)-reduced density matrix relative to the purely factorized (N_1,N_2)-body state $u^{\otimes N_1}\otimes v^{\otimes N_2}$.

By definition, the vanishing of $R_{\psi_N}^{(1,1)}$ in the limit of large N_1 and N_2 implies that ψ_N exhibits condensation in the sense of (1.6). The next two Lemmas (that we already proved in [67]) show that the vanishing of any of the quantities defined in (1.7) and (1.8) is equivalent to the vanishing of all the others, for all k_1,k_2.

Lemma 1.1. *For the quantities defined in* (1.7) *for* $k_1, k_2 \in \{0,1\}$*, one has*

$$\alpha_{\psi_N}^{(1,0)} \leqslant \alpha_{\psi_N}^{(1,1)}\,, \qquad \alpha_{\psi_N}^{(0,1)} \leqslant \alpha_{\psi_N}^{(1,1)} \tag{1.9}$$

and

$$\alpha_{\psi_N}^{(1,1)} \leqslant \alpha_{\psi_N}^{(1,0)} + \alpha_{\psi_N}^{(0,1)}\,. \tag{1.10}$$

Lemma 1.2. *For the quantities defined in* (1.7)-(1.8) *for* $k_j \in \{1,\dots,N_j\}$*,* $j = 1,2$*, one has*

$$\begin{aligned} \alpha_{\psi_N}^{(k_1,k_2)} &\leqslant R_{\psi_N}^{(k_1,k_2)} \leqslant 2\sqrt{\alpha_{\psi_N}^{(k_1,k_2)}} && (1.11)\\ \alpha_{\psi_N}^{(k_1,k_2)} &\leqslant \max\{k_1,k_2\}\cdot\alpha_{\psi_N}^{(1,1)}\,. && (1.12) \end{aligned}$$

The α-indicators will play a crucial role in Chapter 4. They quantify the difference between the maximal possible value 1 and the expectation of the reduced density matrix on the factorized state. The apparently stronger trace norm displacement (the R-indicators) turns out to be equivalent to the former, in view of (1.11).

Lemma 1.1 shows that for the control of the double condensation, simultaneously in each component, one can equivalently monitor the vanishing of $\alpha^{(1,1)}$ or the vanishing of $\alpha^{(1,0)}$ *and* $\alpha^{(0,1)}$. Lemma 1.2 shows in addition that the vanishing of $\alpha^{(1,1)}$ or of higher order α-indicators are also equivalent, with a deterioration (the factor $\max\{k_1,k_2\}$ in (1.12)) that depends on the size of the subsystem of particles in each component on which one monitors the occurrence of condensation.

Proof of Lemma 1.1. If $\{v_n\}_{n=1}^\infty$ is an orthonormal basis of $\mathfrak{h} := L^2(\mathbb{R}^3)$ such that $v_1 = v$, one has

$$\langle u\otimes v\,,\gamma_{\psi_N}^{(1,1)}\,u\otimes v\rangle_{\mathfrak{h}\otimes\mathfrak{h}} \leqslant \sum_{n=1}^{\infty}\langle u\otimes v_n\,,\gamma^{(1,1)}\,u\otimes v_n\rangle_{\mathfrak{h}\otimes\mathfrak{h}} = \langle u\,,\gamma^{(1,0)}u\rangle_{\mathfrak{h}}$$

where the inequality is due to the positivity of $\gamma_{\psi_N}^{(1,1)}$ and in the last identity we used the definition of partial trace. This shows that $\alpha_{\psi_N}^{(1,0)} \leqslant \alpha_{\psi_N}^{(1,1)}$, and analogously $\alpha_{\psi_N}^{(0,1)} \leqslant \alpha_{\psi_N}^{(1,1)}$. To prove (1.10), we exploit the positivity of the projections $\mathbb{1} - |u\rangle\langle u|$ and $\mathbb{1} - |v\rangle\langle v|$, and hence of their tensor product: one finds

$$\begin{aligned} 0 &\leqslant \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big[\,\gamma_{\psi_N}^{(1,1)}(\mathbb{1}_{\mathfrak{h}} - |u\rangle\langle u|)\otimes(\mathbb{1}_{\mathfrak{h}} - |v\rangle\langle v|)\,\big]\\ &= \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big[\,\gamma_{\psi_N}^{(1,1)}(\mathbb{1}_{\mathfrak{h}} - |u\rangle\langle u|)\otimes\mathbb{1}_{\mathfrak{h}}\,\big] + \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big[\,\gamma_{\psi_N}^{(1,1)}\,\mathbb{1}_{\mathfrak{h}}\otimes(\mathbb{1}_{\mathfrak{h}} - |v\rangle\langle v|)\,\big]\\ &\qquad - \mathrm{Tr}_{\mathfrak{h}\otimes\mathfrak{h}}\big[\,\gamma_{\psi_N}^{(1,1)}(\mathbb{1}_{\mathfrak{h}\otimes\mathfrak{h}} - |u\rangle\langle u|\otimes|v\rangle\langle v|)\,\big]\\ &= \alpha_{\psi_N}^{(1,0)} + \alpha_{\psi_N}^{(0,1)} - \alpha_{\psi_N}^{(1,1)} \end{aligned}$$

and the conclusion follows. $\square$

Proof of Lemma 1.2. Inequalities (1.11) are established precisely as in the one-component case, since here one only deals with the rank-one projection $|u^{\otimes k_1}\otimes v^{\otimes k_2}\rangle\langle u^{\otimes k_1}\otimes v^{\otimes k_2}|$ and the density matrix $\gamma_{\psi_N}^{(k_1,k_2)}$ on the (k_1+k_2)-body space $\mathcal{H}_{k_1,k_2}$, with no reference to the two-component structure or to the numbers k_1, k_2 – see, e.g., [44, Lemma 2.3] (the constant 2 in the second inequality in (1.11) is an easy improvement of the constant $2\sqrt{2}$ obtained in [44, Lemma 2.3]). As for (1.12), one first repeats component-wise the very same argument that allows for a control of the k-th marginal in terms of the $(k-1)$-th marginal precisely as in the one-component case [44, Lemma 2.1], thus obtaining

$$\alpha_{\psi_N}^{(k_1,k_2)} \;\leqslant\; \alpha_{\psi_N}^{(k_1-1,k_2-1)} + \alpha_{\psi_N}^{(1,1)} \,.$$

By iteration, and supposing for example $k_1 < k_2$, one gets

$$\alpha_{\psi_N}^{(k_1,k_2)} \;\leqslant\; k_1 \alpha_{\psi_N}^{(1,1)} + \alpha_{\psi_N}^{(0,k_2-k_1)} \,.$$

In turn, for the one-component (k_2-k_1)-marginal $\alpha_{\psi_N}^{(0,k_2-k_1)}$ the standard one-component argument [44, Lemma 2.1] yields

$$\alpha_{\psi_N}^{(0,k_2-k_1)} \;\leqslant\; (k_2-k_1)\, \alpha_{\psi_N}^{(0,1)}$$

and by Lemma 1.1 $\alpha_{\psi_N}^{(0,1)} \leqslant \alpha_{\psi_N}^{(1,1)}$. By combining these inequalities,

$$\alpha_{\psi_N}^{(k_1,k_2)} \;\leqslant\; k_1 \alpha_{\psi_N}^{(1,1)} + (k_2-k_1)\, \alpha_{\psi_N}^{(0,1)} \;\leqslant\; k_2\, \alpha_{\psi_N}^{(1,1)}$$

which proves (1.12). □

1.3 Many-body Hamiltonians, scaling limits, and effective theories

Let us now introduce the models that will be studied in the next Chapters. This is done by specifying the many-body Hamiltonian, an operator on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ which represents the energy of the system and governs the time evolution.

The main results that will be presented are the proof of Bose-Einstein condensation for the ground state, the computation of the ground-state energy asymptotics in the large-N_1, N_2 limit and the proof of persistence of condensation under many-body time evolution.

As presented in the Introduction for the one-component setting, a systematic treatment of such problems in a genuine thermodynamic limit is at the moment not available. Hence, the limit of infinitely many particles requires suitable scaling prescriptions on the many-body Hamiltonian. As customary, this is done by introducing a dependence on the number of particles in the inter-particle interaction.

To be precise, we shall consider the following Hamiltonian operator on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$

$$\begin{aligned} H_N \;:=\; & \sum_{j=1}^{N_1} \big(-\Delta_{x_j} + U_{\mathrm{trap}}^{(1)}(x_j) \big) + \frac{1}{N} \sum_{1\leqslant j<r\leqslant N_1} V_N^{(1)}(x_i - x_j) \\ & + \sum_{k=1}^{N_2} \big(-\Delta_{y_k} + U_{\mathrm{trap}}^{(2)}(y_k) \big) + \frac{1}{N} \sum_{1\leqslant k<\ell\leqslant N_2} V_N^{(2)}(y_k - y_\ell) \\ & + \frac{1}{N} \sum_{j=1}^{N_1} \sum_{k=1}^{N_2} V_N^{(12)}(x_j - y_k)\,, \end{aligned} \tag{1.13}$$

with self-explanatory kinetic, confining, and interaction terms. Depending on the problem under investigation, different assumptions on the functions $U_{\mathrm{trap}}^{(1)}$, $U_{\mathrm{trap}}^{(2)}$, $V_N^{(1)}$, $V_N^{(2)}$, $V_N^{(12)}$ will be made. Such assumptions will always make H_N be unambiguously realized as a self-adjoint operator on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$.

The scaling results in pair potentials $V_N^{(1)}$, $V_N^{(2)}$, and $V_N^{(12)}$ which depend on the number of particles, and in overall N^{-1} coupling constants. Two particular regimes will be considered in the present work: the *mean field* regime, for interactions of weak magnitude and long range, and the *Gross-Pitaevskii* regime, for interactions of strong magnitude and short range. The two regimes correspond to two different specializations of (1.13): the mean field Hamiltonian H_N^{MF} and the Gross-Pitaevskii Hamiltonian H_N^{GP}, in which the interaction potentials $V_N^{(\alpha)}$ are chosen, respectively, as

$$\begin{aligned} V_N^{(\alpha),\mathrm{MF}}(x) \;&:=\; V^{(\alpha)}(x), \\ V_N^{(\alpha),\mathrm{GP}}(x) \;&:=\; N^3 V^{(\alpha)}(Nx), \end{aligned} \qquad \alpha\in\{1,2,12\} \tag{1.14}$$

for suitable N-independent potentials $V^{(1)}$, $V^{(2)}$, and $V^{(12)}$. In fact, it is easy to see what the needed transformation is in order for (1.13)-(1.14) to reproduce the 'physical' mean field and Gross-Pitaevskii scalings that were inferred in [67]:

$$\begin{aligned} \text{mean field:} \qquad & V^{(j)}(x) \;=\; c_j^{-1}\mathcal{V}^{(j)}(x) \\ \text{Gross-Pitaevskii:} \qquad & V^{(j)}(x) \;=\; c_j^{2}\,\mathcal{V}^{(j)}(c_j\,x) \qquad j\in\{1,2\} \\ \text{both:} \qquad & V^{(12)}(x) \;=\; \mathcal{V}^{(12)}(x)\,. \end{aligned} \tag{1.15}$$

One should therefore keep in mind that the physical conditions are on the $\mathcal{V}^{(\alpha)}$'s, although mathematically we shall qualify the $V^{(\alpha)}$'s.

For H_N^{MF} and H_N^{GP}, the ground state energies are defined by

$$\begin{aligned} E_N^{\mathrm{MF}} \;&:=\; \inf\sigma(H_N^{\mathrm{MF}}) \\ E_N^{\mathrm{GP}} \;&:=\; \inf\sigma(H_N^{\mathrm{GP}}). \end{aligned} \tag{1.16}$$

It is worth noticing that our assumptions on the U's and on the V's will always ensure both ground state energies to be finite.

The asymptotic computation of E_N^{GP} and of E_N^{MF} is among the main results of, respectively, Chapter 2 and Chapter 3. It turns out that both quantities are captured, to the leading order in N, by the minima of suitable effective one-body functionals. While leaving to the next Chapters the precise statements and proofs of our main results, we define here the energy functionals of the effective theories corresponding to the two scaling regimes in (1.14).

The relevant effective model for the mean-field regime is a two-component Hartree theory whose energy functional reads

$$\begin{aligned} \mathcal{E}^{\mathrm{H}}[u,v] \;:=\; & c_1\int_{\mathbb{R}^3}|\nabla u|^2\,\mathrm{d}x + c_1\int_{\mathbb{R}^3}U_{\mathrm{trap}}^{(1)}|u|^2\,\mathrm{d}x + \frac{c_1^2}{2}\int_{\mathbb{R}^3}(V^{(1)}*|u|^2)\,|u|^2\,\mathrm{d}x \\ & + c_2\int_{\mathbb{R}^3}|\nabla v|^2\,\mathrm{d}x + c_2\int_{\mathbb{R}^3}U_{\mathrm{trap}}^{(2)}|u|^2\,\mathrm{d}x + \frac{c_2^2}{2}\int_{\mathbb{R}^3}(V^{(2)}*|v|^2)|v|^2\,\mathrm{d}x \\ & + c_1c_2\int_{\mathbb{R}^3}(V^{(12)}*|v|^2)|u|^2\,\mathrm{d}x, \end{aligned} \tag{1.17}$$

where c_1 and c_2 are the population ratios defined in (1.2). The quadratic terms clearly correspond to the single-particle summands of H_N^{MF}, while the non-local quartic terms correspond to the pair potentials. Notice that, depending on the regularity of the potentials $U_{\mathrm{trap}}^{(1)}, U_{\mathrm{trap}}^{(2)}, V^{(1)}, V^{(2)}, V^{(12)}$, the domain of $\mathcal{E}^{\mathrm{H}}$ might vary.

The emergence of the convolution in (1.17) is heuristically explained as a consequence of the law or large numbers. If particles of the first species are distributed according to the density $|u(x)|^2$, then the j-th particle experiences the intra-species interaction energy

$$\frac{1}{N}\sum_{j\neq k} V^{(1)}(x_j - x_k) \;\simeq\; c_1 \int V^{(1)}(x_j - y)|u(y)|^2\,\mathrm{d}y \;\equiv\; c_1(V^{(1)} * |u|^2)(x_j).$$

The emergence of convolutions involving $V^{(2)}$ and $V^{(12)}$ is explained analogously.

In the Gross-Pitaevskii regime, on the other hand, the effective functional depends on the scattering lengths of the pair potentials $V^{(\alpha)}$, $\alpha \in \{1, 2, 12\}$, whose definition we recall here (see [56, Appendix C] for a more detailed presentation).

For a positive, compactly supported and spherically symmetric $V^{(\alpha)}$, consider the solution $f^{(\alpha)}$ to the equation

$$\Big(-\Delta + \frac{V^{(\alpha)}}{2}\Big) f^{(\alpha)} \;=\; 0,$$

with the boundary condition $f^{(\alpha)}(x) \to 1$ for $|x| \to +\infty$. Then, for $|x|$ large enough,

$$f^{(\alpha)}(x) \;=\; 1 - \frac{a_\alpha}{|x|},$$

for an appropriate constant a_α, which is called the scattering length of $V^{(\alpha)}$.

The Gross-Pitaevskii functional then reads

$$\begin{aligned} \mathcal{E}^{\mathrm{GP}}[u,v] \;:=\; & c_1 \int_{\mathbb{R}^3} |\nabla u|^2\,\mathrm{d}x + c_1 \int_{\mathbb{R}^3} U^{(1)}_{\mathrm{trap}}|u|^2\,\mathrm{d}x + 4\pi a_1 c_1^2 \int_{\mathbb{R}^3} |u|^4\,\mathrm{d}x \\ & + c_2 \int_{\mathbb{R}^3} |\nabla v|^2\,\mathrm{d}x + c_2 \int_{\mathbb{R}^3} U^{(2)}_{\mathrm{trap}}|u|^2\,\mathrm{d}x + 4\pi a_2 c_2^2 \int_{\mathbb{R}^3} |v|^4\,\mathrm{d}x \\ & + 8\pi a_{12} c_1 c_2 \int_{\mathbb{R}^3} |v|^2|u|^2\,\mathrm{d}x. \end{aligned} \tag{1.18}$$

Notice that, in $\mathcal{E}^{\mathrm{GP}}$, the details of the functions $V^{(\alpha)}$ do not play a role, and the only relevant parameter for the inter-particle interactions are the scattering lengths.

1.4 Quantum de Finetti theorem

To conclude this Chapter, we state and prove the two-component quantum de Finetti theorem, which will be used in Chapter 2 and 3. It is an abstract result, essentially depending on the structure of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ only, which fixes the asymptotic form of reduced density matrices.

Theorem 1.3 (Quantum de Finetti theorem for 2-component Bose gas)**.** *Let $\mathcal{K}$ be a separable Hilbert space, and let $\{\psi_N\}_N$ be a sequence of wave-functions such that, for every N, ψ_N belongs to $\mathcal{K}^{\otimes_{\mathrm{sym}} N_1} \otimes \mathcal{K}^{\otimes_{\mathrm{sym}} N_2}$ (recall that $N_j = c_j N$, $j = 1, 2$). Then, up to a subsequence of the sequence $\{\psi_N\}_N$, there exists a Borel probability measure μ supported on the set $\{(u,v) : u, v \in \mathcal{K}, \|u\| \leqslant 1, \|v\| \leqslant 1\}$ such that*

$$\gamma^{(k,\ell)}_{\psi_N} \;\rightharpoonup\; \int |u^{\otimes k} \otimes v^{\otimes \ell}\rangle\langle u^{\otimes k} \otimes v^{\otimes \ell}|\,\mathrm{d}\mu(u,v), \quad \forall k, \ell = 0, 1, 2, \ldots \tag{1.19}$$

weakly- in trace class as $N \to \infty$. Moreover, if $\gamma_{\psi_N}^{(1,0)}$ and $\gamma_{\psi_N}^{(0,1)}$ converge strongly in trace class, then μ is supported on the set $\{(u,v) : u, v \in \mathcal{K}, \|u\| = \|v\| = 1\}$ and the convergence in* (1.19) *is strong in trace class for all $k, \ell \geqslant 0$.*

This is the two-component analogue of the quantum de Finetti theorem proved in [92], [41] for the case of strong convergence and in [4], [47] for the case of weak convergence. We sketch here a proof of Theorem 1.3, taken from our work [64], which goes through an adaptation of the strategy used in [47] to treat the one-component case.

First, we state and prove the finite dimensional version of Theorem 1.3. It is the two-component result corresponding to the quantitative quantum de Finetti theorem in [20] (see also [34], [48] and the references therein for related results).

Lemma 1.4 (Quantum de Finetti theorem in finite dimensions)**.** *Let $\mathcal{K}$ be a Hilbert space with $\dim \mathcal{K} = d < +\infty$. Let ψ_N be a wave function in $\mathcal{K}_{\mathrm{sym}}^{\otimes N_1} \otimes \mathcal{K}_{\mathrm{sym}}^{\otimes N_2}$. Then there exists a Borel probability measure μ_N supported on the set*

$$\{(u,v) : u, v \in \mathcal{K}, \|u\| = \|v\| = 1\}$$

such that

$$\operatorname{Tr}\left|\gamma_{\psi_N}^{(k,\ell)} - \int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu_N(u,v)\right| \leqslant Cd\Big(\frac{k_1}{N_1} + \frac{k_2}{N_2}\Big)$$

for all $k_1 \in \{0, 1, 2, ..., N_1\}, k_2 \in \{0, 1, ..., N_2\}$.

Proof. Recall the Schur formula

$$\int_{\|u\|=1} |u^{\otimes N_1}\rangle\langle u^{\otimes N_1}| \mathrm{d}u \;=\; c_{N_1} \mathbb{1}_{\mathcal{K}_{\mathrm{sym}}^{\otimes N_1}}$$

where $\mathrm{d}u$ is the (normalized) Haar measure on the unit sphere $\{u \in \mathcal{K}, \|u\| = 1\}$ and

$$c_{N_1} \;:=\; \dim\left(\mathcal{K}_{\mathrm{sym}}^{\otimes N_1}\right) = \binom{N_1 + d - 1}{d - 1}.$$

From this and a similar identity for $\mathcal{K}_{\mathrm{sym}}^{\otimes N_2}$, we can write

$$\int_{\|u\|=1, \|v\|=1} |u^{\otimes N_1}\rangle\langle u^{\otimes N_1}| \otimes |v^{\otimes N_2}\rangle\langle v^{\otimes N_2}| \,\mathrm{d}u\mathrm{d}v \;=\; c_{N_1} c_{N_2} \mathbb{1}_{\mathcal{K}_{\mathrm{sym}}^{\otimes N_1}} \otimes \mathbb{1}_{\mathcal{K}_{\mathrm{sym}}^{\otimes N_2}}.$$

The latter representation suggests that a natural candidate for μ_N is the Husimi measure

$$\mu_N(u,v) \;=\; c_{N_1} c_{N_2} \left|\langle u^{\otimes N_1} \otimes v^{\otimes N_2}, \psi_N\rangle\right|^2 \mathrm{d}u\mathrm{d}v.$$

The remaining part of the proof is similar to the proof in the one-component case from [20] or [48]. □

Now we are ready to prove Theorem 1.3.

Proof of Theorem 1.3. **Step 1: Finite dimensional case.** We first consider the case in which $\mathcal{K}$ is finite dimensional. By Lemma 1.4, from the wave function ψ_N we can construct a Borel probability measure μ_N supported on the set

$$\{(u,v) : u, v \in \mathcal{K}, \|u\| = \|v\| = 1\}$$

such that

$$\lim_{N\to\infty} \operatorname{Tr}\left|\gamma_{\psi_N}^{(k,\ell)} - \int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu_N(u,v)\right| \;=\; 0, \quad \forall k,\ell = 0,1,2,...$$

Now, $\{\mu_N\}$ is a sequence of Borel probability measures supported on a compact set. Hence, up to a subsequence, μ_N converges to a Borel probability measure μ on $\{(u,v) : u,v \in \mathcal{K}, \|u\| = \|v\| = 1\}$. This ensures that

$$\lim_{N\to\infty} \operatorname{Tr}\left|\gamma_{\psi_N}^{(k,\ell)} - \int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu(u,v)\right| \;=\; 0, \quad \forall k,\ell = 0,1,2,...$$

Step 2: Infinite dimensional case. Suppose now $\mathcal{K}$ is infinite dimensional, and let $\{\varphi_n\}_{n=1}^{\infty}$ be an orthonormal basis of $\mathcal{K}$. Let P_n be the projection onto the subspace $W_n = \operatorname{span}(\varphi_1, ..., \varphi_n)$.

Since the operator $\gamma_{\psi_N}^{(k,\ell)}$ is bounded in trace class uniformly in N, up to a subsequence, we have

$$\gamma_{\psi_N}^{(k,\ell)} \;\rightharpoonup\; \gamma^{(k,\ell)}$$

weakly-* in trace class for all $k, \ell \geqslant 0$. Consequently, for every $n \in \mathbb{N}$ fixed, we have the strong convergence

$$P_n^{\otimes k+\ell}\gamma_{\psi_N}^{(k,\ell)}P_n^{\otimes k+\ell} \;\to\; P_n^{\otimes k+\ell}\gamma^{(k,\ell)}P_n^{\otimes k+\ell}, \quad \forall k,\ell \geqslant 0. \tag{1.20}$$

Now using the geometric localization method in Fock space of [46], we can find a state $\Gamma_{N,n}$ in the Fock space $\mathcal{F}(W_n) \otimes \mathcal{F}(W_n)$, located in the sectors with number of particles not bigger than N, whose reduced density matrices are

$$\Gamma_{N,n}^{(k,\ell)} \;=\; P_n^{\otimes k+\ell}\gamma_{\psi_N}^{(k,\ell)}P_n^{\otimes k+\ell}, \quad \forall\, 0 \leqslant k \leqslant N_1, 0 \leqslant \ell \leqslant N_2.$$

Since W_n is finite dimensional, we can argue as in Step 1 for the state $\Gamma_{N,n}$ to find a Borel probability measure μ_n supported on the set

$$\{(u,v) : u, v \in W_n, \|u\| = \|v\| = 1\}$$

such that

$$\begin{aligned}\lim_{N\to\infty} \operatorname{Tr}\Big| &P_n^{\otimes k+\ell}\gamma_{\psi_N}^{(k,\ell)}P_n^{\otimes k+\ell} \\ &- \left(\operatorname{Tr}\left[P_n^{\otimes k+\ell}\gamma_{\psi_N}^{(k,\ell)}P_n^{\otimes k+\ell}\right]\right)\int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu_n(u,v)\Big| \;=\; 0.\end{aligned} \tag{1.21}$$

From (1.20) and (1.21), we deduce that

$$P_n^{\otimes k+\ell}\gamma^{(k,\ell)}P_n^{\otimes k+\ell} = C_{k,\ell,n}\int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu_n(u,v), \quad \forall k,\ell \geqslant 0, \tag{1.22}$$

where

$$C_{k,\ell,n} = \operatorname{Tr}\Big[P_n^{\otimes k+\ell}\gamma^{(k,\ell)}P_n^{\otimes k+\ell}\Big].$$

Next, note that if $m \geqslant n$, then the measure μ_n is the cylindrical projection $(\mu_m)_{|W_n \oplus W_n}$. Therefore, according to [46, Lemma 1], there exists a Borel probability measure μ supported on

$$\{(u,v) : u, v \in \mathcal{K}, \|u\| \leqslant 1, \|v\| \leqslant 1\}$$

such that for all $n = 1, 2, ...$, the measure μ_n coincides with the cylindrical projection $\mu_{|W_n \oplus W_n}$. Consequently, (1.22) can be rewritten as

$$\begin{aligned} P_n^{\otimes k+\ell}\gamma^{(k,\ell)}P_n^{\otimes k+\ell} &= \int |(P_n u)^{\otimes k}\rangle\langle(P_n u)^{\otimes k}| \otimes |(P_n v)^{\otimes \ell}\rangle\langle(P_n v)^{\otimes \ell}| \mathrm{d}\mu(u,v) \\ &= P_n^{\otimes k+\ell}\Big(\int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu(u,v)\Big)P_n^{\otimes k+\ell}. \end{aligned}$$

Since $P_n \to \mathbb{1}_{\mathcal{K}}$ as $n \to \infty$, we deduce that

$$\gamma^{(k,\ell)} = \int |u^{\otimes k}\rangle\langle u^{\otimes k}| \otimes |v^{\otimes \ell}\rangle\langle v^{\otimes \ell}| \mathrm{d}\mu(u,v), \quad \forall k, \ell \geqslant 0. \tag{1.23}$$

Step 3: Strong convergence. If we assume further that $\gamma_{\psi_N}^{(1,0)}$ and $\gamma_{\psi_N}^{(0,1)}$ converge strongly in trace class, then $\operatorname{Tr}\gamma^{(1,0)} = \operatorname{Tr}\gamma^{(0,1)} = 1$. By taking the trace of (1.23), we get

$$\int \|u\|^2 \mathrm{d}\mu(u,v) = \int \|v\|^2 \mathrm{d}\mu(u,v) = 1.$$

Thus, we conclude that μ is supported on

$$\{(u,v) : u, v \in \mathcal{K}, \|u\| = \|v\| = 1\}.$$

Moreover, again by (1.23), we have $\operatorname{Tr}\gamma^{(k,\ell)} = 1$, and hence $\gamma_N^{(k,\ell)}$ converges to $\gamma^{(k,\ell)}$ strongly in trace class for all $k, \ell \geqslant 0$. $\square$

Chapter 2

Ground state of Bose mixtures in the Gross-Pitaevskii regime

Let H_N^{GP} be the Gross-Pitaevskii Hamiltonian defined by (1.13) and (1.14), and let E_N^{GP} be its ground state energy. In this Chapter we are going to show that under suitable, physically realistic conditions the many-body ground state energy per particle E_N^{GP}/N converges to the minimum of the Gross-Pitaevskii functional (1.18). Moreover, the corresponding many-body ground state exhibits Bose-Einstein condensation in both components on the unique minimizer (u_0, v_0) of the Gross-Pitaevskii functional.

This Chapter is based on my work [64] in collaboration with Michelangeli and Nam.

2.1 Assumptions and main result

We require the following assumptions on the potentials that appear in the many-body Hamiltonian H_N^{GP}.

(A_1^{GP}) For $\alpha \in \{1,2\}$, the confining potentials satisfy $U_{\mathrm{trap}}^{(\alpha)} \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{R})$ and

$$U_{\mathrm{trap}}^{(\alpha)}(x) \to +\infty \quad \text{as} \quad |x| \to +\infty.$$

(A_2^{GP}) For $\alpha \in \{1,2,12\}$ the interaction potentials $V^{(\alpha)} \in C_c^\infty(\mathbb{R}^3)$ are non-negative, spherically symmetric, and such that the respective scattering lengths satisfy

$$a_1 a_2 \geqslant a_{12}^2 \,. \tag{2.1}$$

The assumption (A_1^{GP}) ensures that the one-body operator $T^{(\alpha)} := -\Delta + U_{\mathrm{trap}}^{(\alpha)}$ is bounded from below, and with compact resolvent. The relevant case of harmonic confinement $U_{\mathrm{trap}}^{(\alpha)}(x) = c_\alpha |x|^2$, often used in experiments, clearly satisfies (A_1^{GP}). It is to be remarked that the results presented below can be generalized to the case in which, in H_N^{GP}, the Laplacian $-\Delta$ is replaced by the magnetic Laplacian $(i\nabla + A(x))^2$.

Condition (2.1) in (A_2^{GP}) is needed to ensure that the minimizer of the Gross-Pitaevskii functional is unique. Such condition explicitly emerges in the physical literature and was recognized in experimental observations as a 'miscibility' condition between the two components of the mixture (that is, the interspecies repulsion does not overcome the repulsion among particles of the same type and the two components are spatially mixed); see, e.g., [32], [60, Section 15.2], [36, Section 16.2.1] and [84, Section 21.1]. It is to be remarked that the results below actually hold in a larger generality in which (2.1) is replaced by the condition that the Gross-Pitaevskii functional has a unique minimizer.

The main result of this Chapter describes the leading order behavior of the many-body ground state energy and ground state in the Gross-Pitaevskii regime.

Theorem 2.1 (Leading order in the Gross-Pitaevskii limit). *Let Assumptions (A_1^{GP}) and (A_2^{GP}) be satisfied. Then the following statements hold true.*

(i) There exists a unique minimizer (u_0, v_0) (up to phases) for the variational problem

$$e_{\mathrm{GP}} := \inf_{\substack{u,v \in H^1(\mathbb{R}^3) \\ \|u\|_{L^2}=\|v\|_{L^2}=1}} \mathcal{E}^{\mathrm{GP}}[u,v].$$

(ii) The ground state energy of H_N^{GP} satisfies

$$\lim_{N\to\infty} \frac{E_N^{\mathrm{GP}}}{N} = e_{\mathrm{GP}}. \tag{2.2}$$

(iii) If ψ_N is an approximate ground state of H_N^{GP}, in the sense that

$$\lim_{N\to\infty} \frac{\langle \psi_N, H_N^{\mathrm{GP}} \psi_N \rangle}{N} = e_{\mathrm{GP}},$$

then it exhibits complete Bose-Einstein condensation in both components

$$\lim_{N\to+\infty} \gamma_{\psi_N}^{(k,\ell)} = |u_0^{\otimes k} \otimes v_0^{\otimes \ell}\rangle\langle u_0^{\otimes k} \otimes v_0^{\otimes \ell}|, \quad \forall k,\ell = 0,1,2,..., \tag{2.3}$$

in trace-norm topology.

A few remarks are in order. First, in Theorem 2.1, local integrability of the pair potentials is actually not essential, and the analysis could be extended, for example, to hard sphere potentials. As will be clear in the course of the proof, thanks to Dyson Lemma, one can replace $V_N^{(\alpha)}$ by a potential with a milder scaling behavior (see Lemma 2.3 below). The detailed profile of the potential plays no role in this, and only its scattering length matters.

The short-range assumption on the potential is not crucial either. Theorem 2.1 could be extended to potentials with fast enough decay, by a spatial cut-off and a standard density argument. However, in the following, we will keep the conditions (A_1^{GP}), (A_2^{GP}) to simplify the presentation.

The analogue of Theorem 2.1 for the one-component case has been proven first by Lieb, Seiringer and Yngvason [57] for the convergence of the ground state energy, and by Lieb and Seiringer [53], [52] for the condensation of the ground state. Later, based on quantum de Finetti methods [20], [4], [47], the ground state energy asymptotics and the proof of condensation for the ground state were re-obtained by Nam, Rougerie and Seiringer [74]. Very recently, Boccato, Brennecke, Cenatiempo, and Schlein [12] obtained the optimal convergence rate in the homogeneous case (where the particles are confined in a unit torus, without external potential). We will follow the approach of [74], and adapt it to the multi-component case.

Theorem 2.1 motivates the assumptions that are typically made on the initial data of the dynamical analysis (see our work [77] whose main result is presented in Chapter 4). There, one proves that the mixture preserves double-component condensation in the course of time evolution, if it is prepared at time $t=0$ in a state of condensation *and* provided that the energy per particle of the initial state is captured by the GP energy functional. In the experiments the preparation of the mixture is precisely obtained by letting the system relax onto the many-body ground state (or a low-energy state), then the dynamical experiments starts by perturbing such an initial state, e.g., removing the confinement [36]. Theorem 2.1 provides the rigorous ground for such initial conditions.

The remaining part of this Chapter is devoted to the proof of Theorem 2.1. We will prove (i) in Section 2.2, (ii) in Section 2.3, and (iii) in Section 2.4.

2.2 Proof of existence and uniqueness of the GP minimizer

Under assumptions (A_1^{GP}) and (A_2^{GP}), the existence of minimizers for the Gross-Pitaevskii functional (1.18) follows easily from standard direct methods in calculus of variations. We only focus on the uniqueness part.

For $f,g\geqslant 0$, let us define the auxiliary functional

$$\mathcal{D}^{\mathrm{GP}}[f,g] \;:=\; \mathcal{E}^{\mathrm{GP}}[\sqrt{f},\sqrt{g}]. \tag{2.4}$$

The first step is to show convexity of $\mathcal{D}^{\mathrm{GP}}$, namely

$$\mathcal{D}^{\mathrm{GP}}\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] \;\leqslant\; \frac{\mathcal{D}^{\mathrm{GP}}[f,g]+\mathcal{D}^{\mathrm{GP}}[r,s]}{2}. \tag{2.5}$$

This is easily checked for the summands of $\mathcal{D}^{\mathrm{GP}}$ that contain the kinetic operator (by [51, Theorem 7.8]) and for those that contain the trapping potentials. For the terms containing the interaction potentials, let us consider, in self-explanatory notation, $\mathcal{D}_1^{\mathrm{GP}}$, $\mathcal{D}_2^{\mathrm{GP}}$, $\mathcal{D}_{12}^{\mathrm{GP}}$ as the three summands of $\mathcal{D}^{\mathrm{GP}}$ containing, respectively, a_1, a_2 and a_{12}. We have the identities

$$\begin{aligned}
\frac{\mathcal{D}_1^{\mathrm{GP}}[f,g]+\mathcal{D}_1^{\mathrm{GP}}[r,s]}{2}-\mathcal{D}_1^{\mathrm{GP}}\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] \;&=\; 4\pi a_1 c_1^2\int\Big|\frac{\widehat{f}(k)-\widehat{r}(k)}{2}\Big|^2\,\mathrm{d}k\\
\frac{\mathcal{D}_2^{\mathrm{GP}}[f,g]+\mathcal{D}_2^{\mathrm{GP}}[r,s]}{2}-\mathcal{D}_2^{\mathrm{GP}}\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] \;&=\; 4\pi a_2 c_2^2\int\Big|\frac{\widehat{g}(k)-\widehat{s}(k)}{2}\Big|^2\,\mathrm{d}k\\
\frac{\mathcal{D}_{12}^{\mathrm{GP}}[f,g]+\mathcal{D}_{12}^{\mathrm{GP}}[r,s]}{2}-\mathcal{D}_{12}^{\mathrm{GP}}\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] \;&=\; 8\pi a_{12} c_1 c_2\int\overline{\frac{\widehat{f}(k)-\widehat{r}(k)}{2}}\,\frac{\widehat{g}(k)-\widehat{s}(k)}{2}\,\mathrm{d}k.
\end{aligned} \tag{2.6}$$

By the Cauchy-Schwarz inequality together with (2.1),

$$\begin{aligned}
&4\pi a_1 c_1^2\int\Big|\frac{\widehat{f}(k)-\widehat{r}(k)}{2}\Big|^2\,\mathrm{d}k+4\pi a_2 c_2^2\int\Big|\frac{\widehat{g}(k)-\widehat{s}(k)}{2}\Big|^2\,\mathrm{d}k\\
&\geqslant\; 8\pi a_{12}c_1c_2\int\Big|\frac{\widehat{f}(k)-\widehat{r}(k)}{2}\Big|\cdot\Big|\frac{\widehat{g}(k)-\widehat{s}(k)}{2}\Big|\,\mathrm{d}k,
\end{aligned}$$

and the convexity property (2.5) follows.

Next, let us show that any Gross-Pitaevskii minimizer is positive, up to an overall complex phase. Indeed, let (u_1, v_1) be a Gross-Pitaevskii minimizer. By the diamagnetic inequality [51, Theorem 7.8], $(|u_1|, |v_1|)$ is a Gross-Pitaevskii minimizer too, and we have

$$\int |\nabla u_1(x)|^2 \, \mathrm{d}x \; = \; \int |\nabla |u_1(x)||^2 \, \mathrm{d}x, \qquad \int |\nabla v_1(x)|^2 \, \mathrm{d}x = \int |\nabla |v_1(x)||^2 \, \mathrm{d}x. \tag{2.7}$$

Moreover, by a standard elliptic regularity argument for the Gross-Pitaevskii equation for $(|u_1|, |v_1|)$, it follows that $|u_1|, |v_1| > 0$ pointwise. Due to [51, Theorem 7.8], this strict positivity together with the equalities (2.7), imply that $u_1 = \theta_1 |u_1|$ and $v_1 = \theta_1' |v_1|$ for complex constants θ_1, θ_1'. Thus, up to complex phases, we can assume that $u_1, v_1 > 0$ pointwise.

Next, assume that (u_1, v_1) and (u_2, v_2) are two Gross-Pitaevskii minimizers, with $u_i, v_i > 0$ for $i = 1, 2$. Denote $f_i := |u_i|^2$ and $g_i := |v_i|^2$. Obviously, (f_1, g_1) and (f_2, g_2) are minimizers for $\mathcal{D}^{\mathrm{GP}}[f, g]$ with the constraint $\|f\|_{L^1} = \|g\|_{L^1} = 1$. Combining with the convexity of $\mathcal{D}^{\mathrm{GP}}$, we have the following chain of inequalities

$$0 \; \geqslant \; \frac{\mathcal{D}^{\mathrm{GP}}[f_1, g_1] + \mathcal{D}^{\mathrm{GP}}[f_2, g_2]}{2} - \mathcal{D}^{\mathrm{GP}}\Big[\frac{f_1 + f_2}{2}, \frac{g_1 + g_2}{2}\Big] \; \geqslant \; 0.$$

This implies

$$\frac{\mathcal{D}^{\mathrm{GP}}[f_1, g_1] + \mathcal{D}^{\mathrm{GP}}[f_2, g_2]}{2} \; = \; \mathcal{D}^{\mathrm{GP}}\Big[\frac{f_1 + f_2}{2}, \frac{g_1 + g_2}{2}\Big],$$

and in particular

$$\frac{\langle \sqrt{f_1}, -\Delta \sqrt{f_1} \rangle + \langle \sqrt{f_2}, -\Delta \sqrt{f_2} \rangle}{2} \; = \; \Big\langle \sqrt{\frac{f_1 + f_2}{2}}, -\Delta \sqrt{\frac{f_1 + f_2}{2}} \Big\rangle. \tag{2.8}$$

By [51, Theorem 7.8], the equality (2.8) and the fact that $f_1, f_2 > 0$ imply that f_1 and f_2 are proportional. The normalization condition $\|f_1\|_{L^1} = \|f_2\|_{L^1} = 1$ implies that $f_1 = f_2$, and hence $u_1 = u_2$. The same argument shows $v_1 = v_2$.

2.3 Proof of the energy convergence

2.3.1 Energy upper bound

We will follow ideas developed in [57], adding some modifications. First, let us recall the following result [30, Appendix A.1].

Lemma 2.2. *Let $0 \leqslant V \in C_c^\infty(\mathbb{R}^3)$ be spherically symmetric and with scattering length $a > 0$. Then $N^2 V(N\cdot)$ has scattering length a/N. Moreover, for every constant $\ell > 0$, if N is large enough so as to have $\operatorname{supp} V \subset \{|x| \leqslant N\ell\}$, then there exists a unique ground state $f \geqslant 0$ of the Neumann problem*

$$-\Delta f + \frac{1}{2} N^2 V(N\cdot) f \; = \; \lambda_N f$$

on the ball $|x| \leqslant \ell$, with $f(x) = 1$ on $|x| = \ell$. We can can extend f to $\mathbb{R}^3$ by setting $f(x) = 1$ if $|x| \geqslant \ell$, and hence

$$-\Delta f + \frac{1}{2} N^2 V(N\cdot) f \; = \; \lambda_N f \, \mathbf{1}_{B(0,\ell)} \tag{2.9}$$

on $\mathbb{R}^3$*. Moreover,*

$$\lambda_N \;=\; \frac{3a}{N\ell^3}+\frac{O(1)}{N^2\ell^4}, \quad 0\leqslant 1-f\leqslant \frac{C\,\mathbf{1}(|x|\leqslant \ell)}{N|x|}, \quad |\nabla f|\leqslant \frac{C\,\mathbf{1}(|x|\leqslant \ell)}{N|x|^2}. \tag{2.10}$$

Trial function. Let us introduce the notation

$$\begin{aligned}
(z_1,...,z_N) \;&:=\; (x_1,...,x_{N_1},y_1,...,y_{N_2}), \qquad (2.11)\\
U_i \;&:=\; \begin{cases} U^{(1)}_{\rm trap} & \text{if} \quad i\leqslant N_1,\\ U^{(2)}_{\rm trap} & \text{if} \quad i> N_1,\end{cases}\\
(V_{ij},a_{i,j}) \;&:=\; \begin{cases} (N^2V^{(1)}(N.),a_1) & \text{if} \quad i,j\leqslant N_1,\\ (N^2V^{(2)}(N.),a_2) & \text{if} \quad i,j> N_1,\\ (N^2V^{(12)}(N.),a_{12}) & \text{if} \quad i\leqslant N_1<j \quad \text{or} \quad j\leqslant N_1<i.\end{cases}
\end{aligned}$$

Let $\ell>0$ be a N-independent constant which will be chosen later to be suitably small. For every $i\neq j$, let $(f_{ij},\lambda_{N,ij})$ be the pair (f,λ_N) provided by Lemma 2.2 with $N^2V(N\cdot)$ replaced by V_{ij}.

In the above notation the many-body Hamiltonian reads

$$H_N^{\rm GP} \;=\; \sum_{i=1}^N(-\Delta_{z_i}+U_i(z_i))+\sum_{i<j}^N V_{ij}(z_i-z_j). \tag{2.12}$$

Let us fix two functions $u,v\in C_c^\infty(\mathbb{R}^3)$, not depending on N or ℓ, such that $\|u\|_{L^2}=\|v\|_{L^2}=1$. For every $i=1,2,...,N$ denote

$$u_i \;:=\; \begin{cases} u & \text{if} \quad i\leqslant N_1,\\ v & \text{if} \quad i> N_1.\end{cases} \tag{2.13}$$

Consider the (non-normalized) trial function

$$\psi^{\rm tr}(z_1,...,z_N) \;:=\; \prod_{i=1}^N u_i(z_i)\prod_{j<k}^N f_{jk}(z_j-z_k). \tag{2.14}$$

Notice that we are using the full product $\prod_{j<k}^N f_{jk}(z_j-z_k)$ to capture the short-range correlation, instead of using only a 'nearest-neighbor induction' as in [57] in the one-component case. We found that this strategy is more transparent and flexible, as it does not require bosonic symmetry between particles.

We have

$$E_N^{\rm GP} \;\leqslant\; \frac{\langle \psi^{\rm tr}, H_N^{\rm GP}\psi^{\rm tr}\rangle}{\langle \psi^{\rm tr},\psi^{\rm tr}\rangle}. \tag{2.15}$$

Norm estimates. For every $i=1,2,...,N$, let us denote the z_i-independent function

$$\psi_i^{\rm tr} \;:=\; \frac{\psi^{\rm tr}}{u_i(z_i)\prod_{j\neq i}^N f_{ij}(z_i-z_j)}.$$

Since $0 \leqslant f_{ij} \leqslant 1$, we have the pointwise estimate

$$|\psi^{\mathrm{tr}}| \leqslant |u_i(z_i)||\psi_i^{\mathrm{tr}}|. \tag{2.16}$$

On the other hand, using (2.10) we write

$$1 - \prod_{j\neq i} f_{ij}^2(z_i - z_j) \leqslant \sum_{j\neq i}(1 - f_{ij}^2(z_i - z_j)) \leqslant \sum_{j\neq i} \frac{C\mathbb{1}(|z_i - z_j| \leqslant \ell)}{N|z_i - z_j|}.$$

Thus

$$\begin{aligned} 0 \leqslant |u_i(z_i)|^2|\psi_i^{\mathrm{tr}}|^2 - |\psi^{\mathrm{tr}}|^2 &= \Big(1 - \prod_{j\neq i} f_{ij}^2(z_i - z_j)\Big)|u_i(z_i)|^2|\psi_i^{\mathrm{tr}}|^2 \\ &\leqslant \sum_{j\neq i} \frac{C\|u_i\|_{L^\infty}\mathbb{1}(|z_i - z_j| \leqslant \ell)}{N|z_i - z_j|}|\psi_i^{\mathrm{tr}}|^2, \end{aligned}$$

and an integration of last estimate in all the variables leads to

$$\|\psi_i^{\mathrm{tr}}\|_{L^2}^2 \geqslant \|\psi^{\mathrm{tr}}\|_{L^2}^2 \geqslant (1 - C\ell^2)\|\psi_i^{\mathrm{tr}}\|_{L^2}^2. \tag{2.17}$$

We will choose $\ell > 0$ small enough so as to have $1-C\ell^2$ close enough to 1. Notice that the L^2-norms in the previous formula, and in the following ones, are different from case to case. For example, the norm of ψ_i^{tr} is in the space $L^2(\mathbb{R}^{3(N-1)})$ of function that do not depend on the variable x_i, while the norm of ψ^{tr} is in $L^2(\mathbb{R}^{3N})$.

Similarly, for every $i \neq j$, the (z_i, z_j)-independent function

$$\psi_{ij}^{\mathrm{tr}} := \frac{\psi^{\mathrm{tr}}}{u_i(z_i)u_j(z_j)f_{ij}(z_i - z_j)\prod_{k\neq i,j}^N f_{ik}(z_i - z_k)f_{jk}(z_j - z_k)}$$

satisfies

$$\|\psi_{ij}^{\mathrm{tr}}\|_{L^2}^2 \geqslant \|\psi^{\mathrm{tr}}\|_{L^2}^2 \geqslant (1 - C\ell^2)\|\psi_{ij}^{\mathrm{tr}}\|_{L^2}^2, \tag{2.18}$$

where the norm of ψ_{ij}^{tr} is in the space $L^2(\mathbb{R}^{3(N-2)})$.

Energy estimates. In order to obtain an upper bound for the energy convergence of Theorem 2.1, we show how to estimate all summands of the energy of the trial function (3.11) in terms of the GP functional, at the expense of negligible remainders.

First, we bound the one-body potential energy. For simplicity, let us assume $U_i \geqslant 0$ for all $i = 1, 2, ..., N$ (this technical assumption will be removed at the end). Using (2.16) and (2.17) we can bound

$$\begin{aligned} \int U_i(z_i)|\psi^{\mathrm{tr}}|^2 \,\mathrm{d}z_1 \dots \mathrm{d}z_N &\leqslant \int U_i(z_i)|u_i(z_i)|^2|\psi_i^{\mathrm{tr}}|^2 \,\mathrm{d}z_1 \dots \mathrm{d}z_N \qquad (2.19) \\ &= \left(\int_{\mathbb{R}^3} U_i(z)|u_i(z)|^2 \,\mathrm{d}z\right) \|\psi_i^{\mathrm{tr}}\|_{L^2}^2 \qquad (2.20) \\ &\leqslant \left(\int_{\mathbb{R}^3} U_i(z)|u_i(z)|^2 \,\mathrm{d}z\right) (1 - C\ell^2)^{-1}\|\psi^{\mathrm{tr}}\|_{L^2}^2. \end{aligned}$$

Here the identity follows from the fact that $\psi_i^{\rm tr}$ is independent of z_i.

Next, let us consider the kinetic energy. For every $i = 1, 2, ..., N$, we have

$$\begin{aligned}\int |\nabla_{z_i}\psi^{\rm tr}|^2 \,\mathrm{d}z_1\dots\mathrm{d}z_N &= \int \Big|(\nabla_{z_i}u_i)\frac{\psi^{\rm tr}}{u_i} + \sum_{j\neq i}(\nabla_{z_i}f_{ij})\frac{\psi^{\rm tr}}{f_{ij}}\Big|^2 \,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &= \int |\nabla_{z_i}u_i|^2\frac{|\psi^{\rm tr}|^2}{|u_i|^2}\,\mathrm{d}z_1\dots\mathrm{d}z_N + \sum_{j\neq i}\int |\nabla_{z_i}f_{ij}|^2\frac{|\psi^{\rm tr}|^2}{|f_{ij}|^2}\,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &\quad + 2\mathrm{Re}\sum_{j\neq i}\int \overline{(\nabla_{z_i}u_i)\frac{\psi^{\rm tr}}{u_i}}(\nabla_{z_i}f_{ij})\frac{\psi^{\rm tr}}{f_{ij}}\,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &\quad + 2\mathrm{Re}\sum_{j\neq i\neq k\neq j}\int \overline{(\nabla_{z_i}f_{ij})\frac{\psi^{\rm tr}}{f_{ij}}}(\nabla_{z_i}f_{ik})\frac{\psi^{\rm tr}}{f_{ik}}\,\mathrm{d}z_1\dots\mathrm{d}z_N.\end{aligned} \tag{2.21}$$

Let us show that the cross terms in (2.21) are small. In fact, for all $i \neq j$, using (2.10), (2.16) and (2.17), we can estimate

$$\begin{aligned}\Big|\int \overline{(\nabla_{z_i}u_i)\frac{\psi^{\rm tr}}{u_i}}(\nabla_{z_i}f_{ij})\frac{\psi^{\rm tr}}{f_{ij}}\Big|\,\mathrm{d}z_1\dots\mathrm{d}z_N &\leqslant \int |\psi_i^{\rm tr}|^2|u_i\nabla_{z_i}u_i||\nabla_{z_i}f_{ij}|\,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &\leqslant \|u_i\nabla u_i\|_{L^\infty}\int |\psi_i^{\rm tr}|^2|\nabla_{z_i}f_{ij}(z_i-z_j)|\,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &= \|u_i\nabla u_i\|_{L^\infty}\left(\int_{\mathbb{R}^3}|\nabla_z f_{ij}(z)|\,\mathrm{d}z\right)\|\psi_i^{\rm tr}\|_{L^2}^2 \\ &\leqslant \frac{C\ell}{N}\|\psi_i^{\rm tr}\|_{L^2}^2 \leqslant \frac{C\ell}{N(1-C\ell^2)}\|\psi^{\rm tr}\|_{L^2}^2.\end{aligned} \tag{2.22}$$

Here the identity follows by integrating w.r.t. z_i first (and using again that $\psi_i^{\rm tr}$ is independent of z_i). The constant C may depend on u and v, but it is always independent of N and ℓ. Similarly, for all $i \neq j \neq k \neq i$, we have

$$\begin{aligned}\Big|\int \overline{(\nabla_{z_i}f_{ij})\frac{\psi^{\rm tr}}{f_{ij}}}(\nabla_{z_i}f_{ik})\frac{\psi^{\rm tr}}{f_{ik}}\Big|\,\mathrm{d}z_1\dots\mathrm{d}z_N &\leqslant \int |\psi_{ij}^{\rm tr}|^2|u_i|^2|u_j|^2|\nabla_{z_i}f_{ij}||\nabla_{z_i}f_{ik}|\mathrm{d}z_1\dots\mathrm{d}z_N \\ &\leqslant \|u_i\|_{L^\infty}^2\|u_j\|_{L^\infty}^2\int |\psi_{ij}^{\rm tr}|^2|\nabla_{z_i}f_{ij}(z_i-z_j)||\nabla_{z_i}f_{ik}(z_i-z_k)|\,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &= \|u_i\|_{L^\infty}^2\|u_j\|_{L^\infty}^2\left(\int_{\mathbb{R}^3}|\nabla_z f_{ij}(z)|\,\mathrm{d}z\right)^2\|\psi_{ij}^{\rm tr}\|_{L^2}^2 \\ &\leqslant \frac{C\ell^2}{N^2}\|\psi_{ij}^{\rm tr}\|_{L^2}^2 \leqslant \frac{C\ell^2}{N^2(1-C\ell^2)}\|\psi^{\rm tr}\|_{L^2}^2.\end{aligned}$$

The identity follows by integrating w.r.t. z_j fist, then integrating w.r.t. z_i, and using the fact that $\psi_{ij}^{\rm tr}$ is independent of (z_i, z_j).

Next we turn to the main terms in (2.21). The first term can be estimated similarly to (2.19):

$$\begin{aligned}\int |\nabla_{z_i}u_i|^2\frac{|\psi^{\rm tr}|^2}{|u_i|^2}\,\mathrm{d}z_1\dots\mathrm{d}z_N &\leqslant \int |\nabla_{z_i}u_i|^2|\psi_i^{\rm tr}|\,\mathrm{d}z_1\dots\mathrm{d}z_N \\ &= \|\nabla u_i\|_{L^2}^2\|\psi_i^{\rm tr}\|_{L^2}^2 \leqslant \frac{1}{1-C\ell^2}\|\nabla u_i\|_{L^2}^2\|\psi^{\rm tr}\|_{L^2}^2.\end{aligned} \tag{2.23}$$

The second term in (2.21) will be coupled with the interaction energy. We have

$$
\begin{aligned}
\int |\nabla_{z_i} f_{ij}(z_i-z_j)|^2 \frac{|\psi^{\mathrm{tr}}|^2}{|f_{ij}|^2}\,\mathrm{d}z_1\ldots\mathrm{d}z_N + \frac{1}{2}\int V_{ij}(z_i-z_j)|\psi^{\mathrm{tr}}|^2\,\mathrm{d}z_1\ldots\mathrm{d}z_N \\
\leqslant \int \Big[|\nabla_{z_i} f_{ij}(z_i-z_j)|^2 + \frac{1}{2}V_{ij}(z_i-z_j)|f_{ij}(z_i-z_j)|^2\Big]|u_i(z_i)|^2|u_j(z_j)|^2|\psi^{\mathrm{tr}}_{ij}|^2\,\mathrm{d}z_1\ldots\mathrm{d}z_N \\
= \left(\int_{\mathbb{R}^3\times\mathbb{R}^3} \Phi_{ij}(x-y)|u_i(x)|^2|u_j(y)|^2\,\mathrm{d}x\mathrm{d}y\right)\|\psi^{\mathrm{tr}}_{ij}\|^2_{L^2} \\
\leqslant \left(\int_{\mathbb{R}^3\times\mathbb{R}^3} \Phi_{ij}(x-y)|u_i(x)|^2|u_j(y)|^2\,\mathrm{d}x\mathrm{d}y\right)\frac{1}{1-C\ell^2}\|\psi^{\mathrm{tr}}\|^2_{L^2}
\end{aligned}
$$

where

$$\Phi_{ij}(z) := |\nabla_z f_{ij}(z)|^2 + \frac{1}{2}V_{ij}(z)|f_{ij}(z)|^2.$$

Since Φ_{ij} is supported on $|x|\leqslant\ell$, we can estimate

$$
\begin{aligned}
\Big|\int_{\mathbb{R}^3\times\mathbb{R}^3} \Phi_{ij}(x-y)|u_i(x)|^2|u_j(y)|^2\,\mathrm{d}x\mathrm{d}y - \|\Phi_{ij}\|_{L^1}\int_{\mathbb{R}^3}|u_i(x)|^2|u_j(x)|^2\,\mathrm{d}x\Big| \\
= \Big|\int_{\mathbb{R}^3\times\mathbb{R}^3} \Phi_{ij}(x-y)|u_i(x)|^2\big(|u_j(x)|^2-|u_j(y)|^2\big)\,\mathrm{d}x\mathrm{d}y\Big| \\
\leqslant \sup_{|x-y|\leqslant\ell}\Big||u_j(x)|^2-|u_j(y)|^2\Big|\int_{\mathbb{R}^3\times\mathbb{R}^3}\Phi_{ij}(x-y)|u_i(x)|^2\,\mathrm{d}x\mathrm{d}y \\
\leqslant C\ell\,\|\nabla(|u_j|^2)\|_{L^\infty}\|\Phi_{ij}\|_{L^1}.
\end{aligned}
$$

Moreover, using equation (2.9) for f_{ij}, the fact that $0\leqslant f_{ij}\leqslant 1$, and the estimate (2.10) for the eigenvalue $\lambda_{N,ij}$ we find that

$$
\begin{aligned}
\|\Phi_{ij}\|_{L^1} &= \int_{\mathbb{R}^3}\Big[|\nabla_z f_{ij}(z)|^2 + \frac{1}{2}V_{ij}(z)|f_{ij}(z)|^2\Big]\,\mathrm{d}z \\
&= \lambda_{N,ij}\int_{\mathbb{R}^3}|f_{ij}(z)|^2\,\mathbf{1}(|z|\leqslant\ell)\,\mathrm{d}z \\
&\leqslant \Big(\frac{3a_{i,j}}{N\ell^3}+\frac{C}{N^2\ell^4}\Big)\int_{\mathbb{R}^3}\mathbf{1}(|z|\leqslant\ell)\,\mathrm{d}z \leqslant \frac{4\pi a}{N}+\frac{C}{N^2\ell}.
\end{aligned}
$$

Thus,

$$
\begin{aligned}
\int_{\mathbb{R}^3\times\mathbb{R}^3}\Phi_{ij}(x-y)|u_i(x)|^2|u_j(y)|^2\,\mathrm{d}x\mathrm{d}y &\leqslant (1+C\ell)\|\Phi_{ij}\|_{L^1}\int_{\mathbb{R}^3}|u_i(x)|^2|u_j(x)|^2\,\mathrm{d}x \\
&\leqslant (1+C\ell)\Big(\frac{4\pi a_{i,j}}{N}+\frac{C}{N^2\ell}\Big)\int_{\mathbb{R}^3}|u_i(x)|^2|u_j(x)|^2\,\mathrm{d}x,
\end{aligned}
$$

and hence

$$
\begin{aligned}
\int\Big[|\nabla_{z_i} f_{ij}(z_i-z_j)|^2\frac{|\psi^{\mathrm{tr}}|^2}{|f_{ij}|^2}+\frac{1}{2}V_{ij}(z_i-z_j)|\psi^{\mathrm{tr}}|^2\Big]\,\mathrm{d}z_1\ldots\mathrm{d}z_N \\
\leqslant \frac{1+C\ell}{1-C\ell^2}\Big(\frac{4\pi a_{i,j}}{N}+\frac{C}{N^2\ell}\Big)\Big(\int_{\mathbb{R}^3}|u_i(x)|^2|u_j(x)|^2\,\mathrm{d}x\Big)\|\psi^{\mathrm{tr}}\|^2_{L^2}.
\end{aligned}
\tag{2.24}
$$

Conclusion of the upper bound. Putting (2.19)-(2.24) together we obtain, for every $i = 1, 2, ..., N$,

$$
\begin{aligned}
&\Big\langle \psi^{\rm tr}, \Big(-\Delta_{z_i} + U_i(z_i) + \sum_{j\neq i}^{N} \frac{1}{2} V_{ij}(z_i - z_j)\Big)\psi^{\rm tr}\Big\rangle \|\psi^{\rm tr}\|_{L^2}^{-2} \\
&\qquad\qquad \leqslant \frac{1}{1-C\ell^2}\left(\|\nabla u_i\|_{L^2}^2 + \int_{\mathbb{R}^3} U_i(z)|u_i(z)|^2\,{\rm d}z\right) + \frac{C\ell}{1-C\ell^2} + \frac{C\ell^2}{1-C\ell^2} \\
&\qquad\qquad\quad + \frac{1+C\ell}{1-C\ell^2}\sum_{j\neq i}^{N}\Big(\frac{4\pi a_{i,j}}{N} + \frac{C}{N^2\ell}\Big)\Big(\int_{\mathbb{R}^3}|u_i(x)|^2|u_j(x)|^2\,{\rm d}x\Big).
\end{aligned}
\tag{2.25}
$$

Summing over $i = 1, 2, ..., N$ and using the choice (2.13), we find that

$$
\begin{aligned}
\frac{E_N^{\rm GP}}{N} \leqslant \frac{\langle \psi^{\rm tr}, H_N^{\rm GP}\psi^{\rm tr}\rangle}{N\|\psi^{\rm tr}\|_{L^2}^2} &\leqslant \frac{c_1}{1-C\ell^2}\left(\|\nabla u\|_{L^2}^2 + \int_{\mathbb{R}^3} U^{(1)}_{\rm trap}(x)|u(x)|^2\,{\rm d}x\right) \\
&\quad + \frac{c_2}{1-C\ell^2}\left(\|\nabla v\|_{L^2}^2 + \int_{\mathbb{R}^3} U^{(2)}_{\rm trap}(x)|v(x)|^2\,{\rm d}x\right) \\
&\quad + c_1^2\frac{1+C\ell}{1-C\ell^2}\Big(4\pi a_1 + \frac{C}{N\ell}\Big)\Big(\int_{\mathbb{R}^3}|u(x)|^4\,{\rm d}x\Big) \\
&\quad + c_2^2\frac{1+C\ell}{1-C\ell^2}\Big(4\pi a_2 + \frac{C}{N\ell}\Big)\Big(\int_{\mathbb{R}^3}|v(x)|^4\,{\rm d}x\Big) \\
&\quad + 2c_1c_2\frac{1+C\ell}{1-C\ell^2}\Big(4\pi a_{12} + \frac{C}{N\ell}\Big)\Big(\int_{\mathbb{R}^3}|u(x)|^2|v(x)|^2\,{\rm d}x\Big) \\
&\quad + \frac{C\ell}{1-C\ell^2} + \frac{C\ell^2}{1-C\ell^2}.
\end{aligned}
\tag{2.26}
$$

Taking $N \to +\infty$, and then letting $\ell \to 0$ in (2.26) leads to

$$
\limsup_{N\to\infty} \frac{E_N^{\rm GP}}{N} \leqslant \mathcal{E}^{\rm GP}[u,v]. \tag{2.27}
$$

So far, we have proved (2.27) under the additional assumption that $U^{(\alpha)}_{\rm trap} \geqslant 0$, $\alpha \in \{1,2\}$. In general, if the $U^{(\alpha)}_{\rm trap}$'s have negative parts, we can use (2.19) with U_i replaced by $\max(U_i, -\varepsilon^{-1}) + \varepsilon^{-1} \geqslant 0$, where $\varepsilon > 0$ is a small constant. This gives, instead of (2.27),

$$
\limsup_{N\to\infty} \frac{E_{N,\varepsilon}^{\rm GP}}{N} \leqslant \mathcal{E}_\varepsilon^{\rm GP}[u,v].
$$

where $E^{\rm GP}_{N,\varepsilon}$ and $\mathcal{E}^{\rm GP}_\varepsilon[u,v]$ are, respectively, the many-body ground state energy and the Gross-Pitaevskii functional with $U^{(\alpha)}_{\rm trap}$ replaced by $\max(U^{(\alpha)}_{\rm trap}, -\varepsilon^{-1})$, $\alpha \in \{1,2\}$. We observe that a ε^{-1} summand appears on both sides of the inequality, and hence exactly cancels. Since, by Lebesgue's monotone convergence theorem, $E^{\rm GP}_{N,\varepsilon} \to E^{\rm GP}_N$ and $\mathcal{E}^{\rm GP}_\varepsilon[u,v] \to \mathcal{E}^{\rm GP}[u,v]$ as $\varepsilon \to 0$, we conclude that (2.27) holds true in general.

Optimizing (2.27) over all $u, v \in C_c^\infty(\mathbb{R}^3)$ satisfying $\|u\|_{L^2} = \|v\|_{L^2} = 1$, we obtain the desired upper bound

$$
\limsup_{N\to\infty} \frac{E_N^{\rm GP}}{N} \leqslant e_{\rm GP}. \tag{2.28}
$$

2.3.2 Dyson Lemma

We now prove the lower bound. We will follow the strategy in [74] and modify it in order to account for the two components. Following ideas from [57], [55], [52], [74], we will replace the short-range potentials $V_N^{(\alpha)}$ by longer range potentials with less singular scaling behavior. This idea goes back to Dyson [26].

For every $R > 0$ define

$$\theta_R(x) \;=\; \theta\Big(\frac{x}{R}\Big), \qquad U_R(x) \;=\; \frac{1}{R^3}U\Big(\frac{x}{R}\Big)$$

where $\theta, U \in C_c^\infty(\mathbb{R}^3)$ are radial functions satisfying

$$0 \;\leqslant\; \theta \;\leqslant\; 1, \qquad \theta(x) \;\equiv\; 0 \text{ for } |x| \;\leqslant\; 1, \qquad \theta(x) \;\equiv\; 1 \text{ for } |x| \;\geqslant\; 2,$$

$$U \geqslant 0, \qquad U(x) \equiv 0 \text{ for } |x| \notin [1/2, 1], \qquad \int_{\mathbb{R}^3} U = 4\pi.$$

We will always denote by $p = -\mathrm{i}\,\nabla$ the momentum coordinate.

The following result is taken from [55].

Lemma 2.3 (Generalized Dyson lemma)**.** *Let v be a non-negative smooth function, supported on $|x| \leqslant R/2$ with scattering length a. Then for all $\varepsilon, s > 0$,*

$$p\theta_s(p)\mathbb{1}(|x| \leqslant R)\theta_s(p)p + \frac{1}{2}v(x) \;\geqslant\; (1-\varepsilon)aU_R(x) - \frac{CaR^2}{\varepsilon s^5}.$$

Proof. The bound follows from [55, Lemma 4] with (U, χ, s) replaced by (U_R, θ_s, s^{-1}) and the first estimate in [55, Eq. (52)]. □

Next, we apply Lemma 2.3 to derive a lower bound to the many-body Hamiltonian H_N^{GP}. Under the notation (2.11), we have

Lemma 2.4 (Lower bound for many-body Hamiltonian)**.** *Let $\varepsilon, s > 0$ be independent of N and let $N^{-1} \ll R \ll N^{-1/2}$. Then*

$$\begin{aligned} H_N^{\mathrm{GP}} \;\geqslant\; & \sum_{i=1}^N \Big[-\Delta_{z_i} + U_i(z_i) - (1-\varepsilon)p_{z_i}^2\theta_s^2(p_{z_i})\Big] \\ & + \frac{(1-\varepsilon)^2}{N}\sum_{j\neq i}^N a_{i,j}U_R(z_i - z_j)\prod_{k\neq i,j}^N \theta_{2R}(z_j - z_k) + o(N). \end{aligned} \tag{2.29}$$

The purpose of Lemma 2.4 is to replace the short-range potentials $V_N^{(\alpha)}$ by the longer range potential U_R, which scales in a mean-field like way. This is done by using almost all of the high-momentum part $p^2\theta_s(p)$ of the kinetic operator, and employing a many-body cut-off $\prod_{k\neq i,j}^N \theta_{2R}(z_j - z_k)$ which rules out the event of having three particles close to each other. This technical cut-off will be removed later.

Proof. We start by noticing that $N^{-1}V_N^{(1)} = N^2 V^{(1)}(N\cdot)$ is supported on $|x| \leqslant CN^{-1}$ and has scattering length $a_1 N^{-1}$. Therefore, when $N^{-1} \ll R \ll N^{-1/2}$ we can apply Lemma 2.3 to obtain

$$p_{z_i}\theta_s(p_{z_i})\mathbb{1}(|z_i - z_j| \leqslant R)\theta_s(p_{z_i})p_{z_i} + \frac{1}{2}V_{ij}(z_i - z_j) \ \geqslant\ (1-\varepsilon)\frac{a_{i,j}}{N}U_R(z_i - z_j) + o(N^{-2}). \quad (2.30)$$

For every $i = 1, 2, ..., N$, if every point in $\{z_j\}_{j\neq i}$ has a distance $\geqslant 2R$ to the others, then there is at most one of them whose distance from z_i is not larger than R. In this case,

$$\sum_{j\neq i}^{N} \mathbb{1}(|z_i - z_j| \leqslant R) \ \leqslant\ 1,$$

and hence summing (2.30) over j leads to

$$p_{z_i}^2\theta_s^2(p_{z_i}) + \sum_{j\neq i}^{N}\frac{1}{2}V_{ij}(z_i - z_j) \ \geqslant\ (1-\varepsilon)\sum_{j\neq i}^{N}\frac{a_{i,j}}{N}U_R(z_i - z_j) + o(N^{-2}).$$

The latter estimate can be extended to all $\{z_j\}_{j\neq i} \subset \mathbb{R}^3$ as

$$p_{z_i}^2\theta_s^2(p_{z_i}) + \sum_{j\neq i}^{N}\frac{1}{2}V_{ij}(z_i - z_j) \ \geqslant\ \frac{(1-\varepsilon)}{N}\sum_{j\neq i}^{N} a_{i,j}U_R(z_i - z_j)\prod_{k\neq i,j}^{N}\theta_{2R}(z_j - z_k) + o(N^{-2}) \quad (2.31)$$

because the left-hand side is always nonnegative. Multiplying both sides by $(1-\varepsilon)$ leads to the desired estimate. □

We use again the notation $(z_1, ..., z_N) := (x_1, ..., x_{N_1}, y_1, ..., y_{N_2})$ and introduce

$$\begin{aligned}
h_i \ &:= \ \begin{cases} \widetilde{T}_{z_i}^{(1)} := -\Delta_{z_i} + U_{\mathrm{trap}}^{(1)}(z_i) - (1-\varepsilon)p_{z_i}^2\theta_s^2(p_{z_i}), & \text{if } i \leqslant N_1, \\ \widetilde{T}_{z_i}^{(2)} := -\Delta_{z_i} + U_{\mathrm{trap}}^{(2)}(z_i) - (1-\varepsilon)p_{z_i}^2\theta_s^2(p_{z_i}) & \text{if } i > N_1, \end{cases} \\
W_i \ &:= \ (1-\varepsilon)^2\sum_{j\neq i}^{N} a_{i,j}U_R(z_i - z_j)\prod_{k\neq i,j}^{N}\theta_{2R}(z_j - z_k), \\
\widetilde{H}_N^{\mathrm{GP}} \ &:= \ \sum_{i=1}^{N}\Big(h_i + \frac{1}{N}W_i\Big).
\end{aligned}$$

Lemma 2.4 is then rewritten as

$$H_N^{\mathrm{GP}} \ \geqslant\ \widetilde{H}_N^{\mathrm{GP}} + o(N). \quad (2.32)$$

Thus, for the lower bound on E_N^{GP}, it suffices to estimate the ground state energy of the modified Hamiltonian $\widetilde{H}_N^{\mathrm{GP}}$.

By proceeding exactly as in [74, Lemma 3.1, Lemma 3.4] (where the symmetries of h_i's and W_i's are not essential), one obtains the second moment estimate

$$(\widetilde{H}_N^{\mathrm{GP}})^2 \ \geqslant\ \frac{1}{3}\Big(\sum_{i=1}^{N} h_i\Big)^2 - C_{\varepsilon,s}N^2. \quad (2.33)$$

This allows us to remove the cut-off $\prod_{k\neq i,j}^{N}\theta_{2R}(z_j-z_k)$ and obtain

$$\widetilde{H}_N^{\mathrm{GP}} \geqslant \sum_{i=1}^{N} h_i + \frac{(1-\varepsilon)^2}{N}\sum_{j\neq i}^{N} a_{i,j}U_R(z_i-z_j) + o(N)(N^{-1}\widetilde{H}_N^{\mathrm{GP}})^4, \tag{2.34}$$

provided that $\varepsilon, s > 0$ are independent of N and $N^{-2/3} \ll R \ll N^{-1/2}$.

Now let $\widetilde{\psi}_N$ be a ground state for $\widetilde{H}_N^{\mathrm{GP}}$ (which exists by a standard compactness argument). Taking the expectation of (2.34) against $\widetilde{\psi}_N$, and using the equation $\widetilde{H}_N^{\mathrm{GP}}\widetilde{\psi}_N = \widetilde{E}_N\widetilde{\psi}_N$ with $\widetilde{E}_N = O(N)$, we find that

$$\begin{aligned}\frac{E_N^{\mathrm{GP}}}{N} &\geqslant \frac{\widetilde{E}_N}{N} + o(1)_{N\to\infty}\\ &\geqslant \left\langle \widetilde{\psi}_N, \left(\frac{1}{N}\sum_{i=1}^{N} h_i + \frac{(1-\varepsilon)^2}{N^2}\sum_{j\neq i}^{N} a_{i,j}U_R(z_i-z_j)\right)\widetilde{\psi}_N\right\rangle + o(1)_{N\to\infty},\end{aligned} \tag{2.35}$$

where the first inequality is due to (2.32). Thus, it remains to bound from below the right-hand side of (2.35).

2.3.3 Energy lower bound

A further simplification on the right-hand side of (2.35) is obtained by inserting a finite dimensional cut-off (similarly to what is done in [74]). We report here the argument.

There exists a constant $C_0 > 0$ (which might depend on s, ε) such that the operator

$$K := \varepsilon(-\Delta) + \min(U_{\mathrm{trap}}^{(1)}, U_{\mathrm{trap}}^{(2}) + C_0$$

satisfies $K \geqslant \mathbb{1}$. Moreover, K has compact resolvent because $\min(U_{\mathrm{trap}}^{(1)}(x), U_{\mathrm{trap}}^{(2)}(x)) \to +\infty$ as $|x| \to +\infty$. Therefore, for every fixed $L > 0$, the spectral projection

$$P := \mathbf{1}(K \leqslant L)$$

has finite rank.

Using the operator inequality (see, e.g. [74, Lemma 3.2])

$$U_R(z_i-z_j) \leqslant C\|U_R\|_{L^1}(1-\Delta_{z_i})^{1-\delta}(1-\Delta_{z_j})^{1-\delta}, \qquad \forall\,\delta\in\left(0,\frac{1}{4}\right) \tag{2.36}$$

and the fact that $1-\Delta$ is K-bounded, one obtains the Cauchy-Schwarz type inequality (see also [74, Eq. before (4.10)])

$$U_R(z_i-z_j) \geqslant P_{z_i}\otimes P_{z_j}U_R(z_i-z_j)P_{z_i}\otimes P_{z_j} - C_{\varepsilon,s}L^{-1/10}K_{z_i}K_{z_j}, \quad \forall\; i\neq j \;\text{ s.t. }\; i,j\in\{1,\dots,N\}.$$

From the second moment estimate (2.33), it follows that

$$\langle\widetilde{\psi}_N, K_{z_i}K_{z_j}\widetilde{\psi}_N\rangle \leqslant C_{\varepsilon,s}, \quad \forall\; i\neq j \;\text{ s.t. }\; i,j\in\{1,\dots,N\}. \tag{2.37}$$

Thus, (2.35) reduces to

$$
\begin{aligned}
\frac{E_N^{\mathrm{GP}}}{N} \geqslant & \left\langle \widetilde{\psi}_N, \left(\frac{1}{N}\sum_{i=1}^N h_i + \frac{(1-\varepsilon)^2}{N^2}\sum_{j\neq i}^N a_{i,j} P_{z_i}\otimes P_{z_j} U_R(z_i - z_j) P_{z_i}\otimes P_{z_j} \right) \widetilde{\psi}_N \right\rangle \\
& + o(1)_{N\to\infty} + O(L^{-1/10}) \\
& = c_1 \operatorname{Tr}\left[\widetilde{T}^{(1)} \gamma^{(1,0)}_{\widetilde{\psi}_N} \right] + c_2 \operatorname{Tr}\left[\widetilde{T}^{(2)} \gamma^{(0,1)}_{\widetilde{\psi}_N} \right] + o(1)_{N\to\infty} + O(L^{-1/10}) \\
& + (1-\varepsilon)^2 c_1^2 a_1 \operatorname{Tr}\left[P_{x_1}\otimes P_{x_2} U_R(x_1-x_2) P_{x_1}\otimes P_{x_2} \gamma^{(2,0)}_{\widetilde{\psi}_N} \right] \\
& + (1-\varepsilon)^2 c_2^2 a_2 \operatorname{Tr}\left[P_{y_1}\otimes P_{y_2} U_R(y_1-y_2) P_{y_1}\otimes P_{y_2} \gamma^{(0,2)}_{\widetilde{\psi}_N} \right] \\
& + (1-\varepsilon)^2 2 c_1 c_2 a_{12} \operatorname{Tr}\left[P_{x}\otimes P_{y} U_R(x-y) P_{x}\otimes P_{y} \gamma^{(1,1)}_{\widetilde{\psi}_N} \right].
\end{aligned}
\tag{2.38}
$$

For the last equality we have used the definition of reduced density matrices (1.3).

The bound is then concluded by an application of the Quantum de Finetti Theorem 1.3. Since

$$
h_i \geqslant K_{z_i} - 2C_{\varepsilon,s}, \quad \forall i = 1, ..., N,
$$

we deduce from (2.37) that $\operatorname{Tr}[K\gamma^{(1,0)}_{\widetilde{\psi}_N}]$ and $\operatorname{Tr}[K\gamma^{(0,1)}_{\widetilde{\psi}_N}]$ are bounded uniformly in N. Since K has compact resolvent, up to a subsequence as $N\to\infty$, we obtain that $\gamma^{(1,0)}_{\widetilde{\psi}_N}$ and $\gamma^{(0,1)}_{\widetilde{\psi}_N}$ converge strongly in trace class. Thus, up to a subsequence again, Theorem 1.3 ensures the existence of a Borel probability measure ν supported on the set

$$
\{(u,v) : u, v \in L^2(\mathbb{R}^3), \|u\|_{L^2} = \|v\|_{L^2} = 1\}
$$

such that, for every $k, \ell \in \mathbb{N}$,

$$
\lim_{N\to\infty} \gamma^{(k,\ell)}_{\widetilde{\psi}_N} = \int |u^{\otimes k}\otimes v^{\otimes \ell}\rangle\langle u^{\otimes k}\otimes v^{\otimes \ell}| \, \mathrm{d}\nu(u,v). \tag{2.39}
$$

We now take the limit $N\to\infty$ in the right side of (2.38), and then the limit $L\to\infty$. Since $\widetilde{T}^{(1)}, \widetilde{T}^{(2)}$ are bounded from below, we can use (2.39) and Fatou's lemma to get

$$
\liminf_{N\to\infty} \operatorname{Tr}\left[\widetilde{T}^{(1)}\gamma^{(1,0)}_{\widetilde{\psi}_N} \right] \geqslant \int \langle u, \widetilde{T}^{(1)} u\rangle \, \mathrm{d}\nu(u,v), \tag{2.40}
$$

$$
\liminf_{N\to\infty} \operatorname{Tr}\left[\widetilde{T}^{(2)}\gamma^{(0,1)}_{\widetilde{\psi}_N} \right] \geqslant \int \langle v, \widetilde{T}^{(2)} v\rangle \, \mathrm{d}\nu(u,v). \tag{2.41}
$$

The operator inequality (2.36) and the fact that $(1-\Delta)$ is K-bounded ensure that $P_x\otimes P_y U_R(x-y)P_x\otimes P_y$ is uniformly bounded in N as an operator. Therefore, the trace class convergence (2.39) implies that

$$
\begin{aligned}
& \operatorname{Tr}\left[P_x \otimes P_y \, U_R(x-y) P_x\otimes P_y \gamma^{(1,1)}_{\widetilde{\psi}_N} \right] \\
& \quad = \int \langle u\otimes v, P_x\otimes P_y \, U_R(x-y) P_x \otimes P_y u\otimes v\rangle \, \mathrm{d}\nu(u,v) + o(1)_{N\to\infty}.
\end{aligned}
$$

From the choice of U_R, we get

$$\lim_{N\to\infty}\langle u\otimes v, P_x\otimes P_y\, U_R(x-y)P_x\otimes P_y u\otimes v\rangle \;=\; \lim_{N\to\infty}\left\langle\, |Pu|^2, U_R * |Pv|^2\,\right\rangle$$
$$= 4\pi\int_{\mathbb{R}^3}|Pu(x)|^2|Pv(x)|^2\,\mathrm{d}x.$$

Next we take the limit $L\to\infty$ to remove the cut-off $P=\mathbf{1}(K\leqslant L)$. Since $\mathrm{Tr}[K\gamma^{(1,0)}_{\widetilde{\psi}_N}]$ and $\mathrm{Tr}[K\gamma^{(0,1)}_{\widetilde{\psi}_N}]$ are bounded, ν is supported on $\mathcal{D}[K]\times\mathcal{D}[K]$ where $\mathcal{D}[K]$ is the quadratic form domain of K. Consequently, for all (u,v) in the support of ν, we have $Pu\to u$ and $Pv\to v$ strongly in $\mathcal{D}[K]$ as $L\to\infty$. Moreover, since $(1-\Delta)$ is K-bounded, we have the continuous embeddings $\mathcal{D}[K]\subset H^1(\mathbb{R}^3)\subset L^4(\mathbb{R}^3)$. Therefore,

$$\lim_{L\to\infty}\int_{\mathbb{R}^3}|Pu(x)|^2|Pv(x)|^2\,\mathrm{d}x \;=\; \int_{\mathbb{R}^3}|u(x)|^2|v(x)|^2\,\mathrm{d}x,$$

and hence

$$\lim_{L\to\infty}\lim_{N\to\infty}\langle u\otimes v, P_x\otimes P_yU_R(x-y)P_x\otimes P_y u\otimes v\rangle \;=\; 4\pi\int_{\mathbb{R}^3}|u(x)|^2|v(x)|^2\,\mathrm{d}x.$$

Thus, by Fatou's lemma, we find that

$$\begin{aligned}&\liminf_{L\to\infty}\liminf_{N\to\infty}\mathrm{Tr}\left[P_x\otimes P_yU_R(x-y)P_x\otimes P_y\gamma^{(1,1)}_{\widetilde{\psi}_N}\right]\\ &\qquad= \liminf_{L\to\infty}\liminf_{N\to\infty}\int\langle u\otimes v, P_x\otimes P_yU_R(x-y)P_x\otimes P_y u\otimes v\rangle\,\mathrm{d}\nu(u,v)\\ &\qquad\geqslant \int\left[4\pi\int_{\mathbb{R}^3}|u(x)|^2|v(x)|^2\,\mathrm{d}x\right]\mathrm{d}\nu(u,v).\end{aligned}\tag{2.42}$$

Similarly, we also have

$$\liminf_{L\to\infty}\liminf_{N\to\infty}\mathrm{Tr}\left[P_{x_1}\otimes P_{x_2}U_R(x_1-x_2)P_{x_1}\otimes P_{x_2}\gamma^{(2,0)}_{\widetilde{\psi}_N}\right] \;\geqslant\; \int\left[4\pi\int_{\mathbb{R}^3}|u(x)|^4\mathrm{d}x\right]\mathrm{d}\nu(u,v),\tag{2.43}$$

$$\liminf_{L\to\infty}\liminf_{N\to\infty}\mathrm{Tr}\left[P_{y_1}\otimes P_{y_2}U_R(y_1-y_2)P_{y_1}\otimes P_{y_2}\gamma^{(0,2)}_{\widetilde{\psi}_N}\right] \;\geqslant\; \int\left[4\pi\int_{\mathbb{R}^3}|v(y)|^4\mathrm{d}x\right]\mathrm{d}\nu(u,v).\tag{2.44}$$

Inserting (2.40)-(2.44) into the right side of (2.38), we arrive at

$$\liminf_{N\to\infty}\frac{E^{\mathrm{GP}}_N}{N} \;\geqslant\; \int\widetilde{\mathcal{E}}^{\mathrm{GP}}_{\varepsilon,s}[u,v]\,\mathrm{d}\nu(u,v) \;\geqslant\; \inf_{\|u\|_{L^2}=\|v\|_{L^2}=1}\widetilde{\mathcal{E}}^{\mathrm{GP}}_{\varepsilon,s}[u,v],\tag{2.45}$$

where

$$\begin{aligned}\widetilde{\mathcal{E}}^{\mathrm{GP}}_{\varepsilon,s}[u,v] \;&:= c_1\langle u,\widetilde{T}^{(1)}u\rangle + c_2\langle v,\widetilde{T}^{(2)}v\rangle + (1-\varepsilon)^2 4\pi a_1 c_1^2\int_{\mathbb{R}^3}|u(x)|^4\,\mathrm{d}x\\ &\quad + (1-\varepsilon)^2 4\pi a_2 c_2^2\int_{\mathbb{R}^3}|v(x)|^4\,\mathrm{d}x + (1-\varepsilon)^2 8\pi a_{12}c_1c_2\int_{\mathbb{R}^3}|u(x)|^2|v(x)|^2\,\mathrm{d}x.\end{aligned}$$

Finally, we take $s\to 0$, and then $\varepsilon\to 0$. By a standard compactness argument as in [52, after (103)], we have

$$\lim_{\varepsilon\to 0}\lim_{s\to 0}\inf_{\|u\|_{L^2}=\|v\|_{L^2}=1}\widetilde{\mathcal{E}}^{\mathrm{GP}}_{\varepsilon,s}[u,v] \;=\; e_{\mathrm{GP}}.\tag{2.46}$$

Thus, (2.45) leads to the desired lower bound

$$\liminf_{N\to\infty} \frac{E_N^{\mathrm{GP}}}{N} \;\geqslant\; e_{\mathrm{GP}}. \tag{2.47}$$

Strictly speaking, we have so far proved (2.47) for a subsequence as $N \to \infty$. However, since the limit e_{GP} is independent of the subsequence, we obtain the estimate for the whole sequence by a standard contradiction argument.

Combining with the energy upper bound (2.28), we conclude the proof of (ii):

$$\lim_{N\to\infty} \frac{E_N^{\mathrm{GP}}}{N} \;=\; e_{\mathrm{GP}}.$$

2.4 Proof of BEC for approximate ground states

Let ψ_N be an approximate ground state for H_N^{GP}. Since $\mathrm{Tr}[(-\Delta + U_{\mathrm{trap}}^{(1)})\gamma_{\psi_N}^{(1,0)}]$ and $\mathrm{Tr}[(-\Delta + U_{\mathrm{trap}}^{(2)})\gamma_{\psi_N}^{(0,1)}]$ are bounded uniformly in N, then, up to a subsequence as $N \to \infty$, $\gamma_{\psi_N}^{(1,0)}$ and $\gamma_{\psi_N}^{(0,1)}$ converge strongly in trace class. Thus, by Theorem 1.3, up to a subsequence again, there exists a Borel probability measure μ supported on the set

$$\{(u,v) : u, v \in L^2(\mathbb{R}^3), \|u\|_{L^2} = \|v\|_{L^2} = 1\}$$

such that, for all $k, \ell \in \mathbb{N}$,

$$\lim_{N\to\infty} \gamma_{\psi_N}^{(k,\ell)} \;=\; \int |u^{\otimes k} \otimes v^{\otimes \ell}\rangle\langle u^{\otimes k} \otimes v^{\otimes \ell}| \,\mathrm{d}\mu(u,v) \tag{2.48}$$

strongly in trace class.

Let us show that μ is supported on the set $\{(e^{i\theta_1}u_0, e^{\theta_2}v_0) : \theta_1, \theta_2 \in \mathbb{R}\}$, where (u_0, v_0) is the unique Gross-Pitaevskii minimizer. This follows from the convergence of ground state energy and, as in [52], from a Hellmann-Feynman type argument that we repeat and adapt to the two-component setting.

Let us define the projector

$$Q \;:=\; |u_0 \otimes v_0\rangle\langle u_0 \otimes v_0|$$

and for every fixed $\eta > 0$, consider the perturbed Hamiltonian

$$H_{N,\eta}^{\mathrm{GP}} \;:=\; H_N^{\mathrm{GP}} + \frac{\eta}{N c_1 c_2} \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} Q_{x_i,y_j},$$

where Q_{x_i,y_j} indicates the projector Q acting on the i-th variable of the first sector of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ and on the j-th variable of the second sector.

Then, by repeating the proof in Section 2.3, we obtain the analogue of (2.2) (a lower bound is sufficient for our purpose)

$$\liminf_{N\to\infty} \frac{\inf \sigma(H_{N,\eta}^{\mathrm{GP}})}{N} \;\geqslant\; \inf_{\|u\|_{L^2} = \|v\|_{L^2} = 1} \Big\{ \mathcal{E}^{\mathrm{GP}}[u,v] + \eta |\langle u, u_0\rangle|^2 |\langle v, v_0\rangle|^2 \Big\} \;=:\; e_{\mathrm{GP},\eta}. \tag{2.49}$$

Next, we write

$$\mathrm{Tr}[Q\gamma_{\psi_N}^{(1,1)}] \;=\; \frac{1}{N^2c_1c_2}\Big\langle\psi_N,\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}Q_{x_i,y_j}\psi_N\Big\rangle \;=\; \frac{1}{N\eta}\Big[\langle\psi_N,H_{N,\eta}^{\mathrm{GP}}\psi_N\rangle-\langle\psi_N,H_N^{\mathrm{GP}}\psi_N\rangle\Big].$$

Using the lower bound (2.49) and the assumption that ψ_N is an approximate ground state for H_N^{GP}, we find that

$$\liminf_{N\to\infty}\mathrm{Tr}[Q\gamma_{\psi_N}^{(1,1)}] \;\geqslant\; \frac{1}{\eta}\Big[e_{\mathrm{GP},\eta}-e_{\mathrm{GP}}\Big].$$

Moreover, we notice that, as $\eta\to 0$, the minimizer (u_η,v_η) corresponding to the variational problem in (2.49) is a minimizing sequence for $\mathcal{E}_{\mathrm{GP}}$ which converges to the unique minimizer (u_0,v_0) of $\mathcal{E}_{\mathrm{GP}}$ by a standard compactness argument. Therefore,

$$\liminf_{\eta\to 0}\frac{1}{\eta}\Big[e_{\mathrm{GP},\eta}-e_{\mathrm{GP}}\Big] \;\geqslant\; \liminf_{\eta\to 0}|\langle u_\eta,u_0\rangle|^2|\langle v_\eta,v_0\rangle|^2 \;=\; 1.$$

This proves that

$$\liminf_{N\to\infty}\mathrm{Tr}[Q\gamma_{\psi_N}^{(1,1)}] \;\geqslant\; 1.$$

By last estimate, the convergence (2.48) implies

$$\int|\langle u,u_0\rangle|^2|\langle v,v_0\rangle|^2\,\mathrm{d}\mu(u,v) \;\geqslant\; 1.$$

Thus, μ is supported on the set $\{(e^{i\theta_1}u_0,e^{\theta_2}v_0):\theta_1,\theta_2\in\mathbb{R}\}$, and hence (2.48) reduces to the desired convergence (2.3):

$$\lim_{N\to\infty}\gamma_{\psi_N}^{(k,\ell)} \;=\; |u_0^{\otimes k}\otimes v_0^{\otimes\ell}\rangle\langle u_0^{\otimes k}\otimes v_0^{\otimes\ell}|,\quad \forall k,\ell=0,1,2,...$$

in trace class. Again, we have so far proved (2.3) for a subsequence as $N\to\infty$, but since the limit does not depend on the subsequence, the convergence actually holds for the whole sequence.

Chapter 3

Ground state of Bose mixtures in the mean-field regime

In this Chapter we qualify an amount of properties of the mean-field Hamiltonian H_N^{MF} defined by (1.13) and (1.14), and of its ground state energy E_N^{MF}. The interest in the present investigation relies on the fact that, compared with Chapter 2, we are able to prove additional properties of H_N^{MF} with respect to the leading-order behavior.

In particular, we shall show that there exists a N-independent self-adjoint operator $\mathbb{H}$ on a suitable Fock space such that

$$E_N^{\mathrm{MF}} \;=\; Ne_{\mathrm{H}} + \inf \sigma(\mathbb{H}) + o(1)_{N\to+\infty}, \tag{3.1}$$

where e_{H} is the minimum of the Hartree functional defined in (1.17). The operator $\mathbb{H}$, called Bogoliubov Hamiltonian, will be introduced in Section 3.1, and is explicitly characterized as the second quantization of the Hessian of the Hartree functional evaluated on the minimizer. Moreover, we will obtain an approximation for the ground state of H_N^{MF} in the norm topology of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$. This is of course much stronger than convergence of reduced density matrices.

The results presented in this Chapter are based on my work [64] in joint collaboration with Michelangeli and Nam.

3.1 Assumptions and main result

We will require the following assumptions on the potentials appearing in the many-body Hamiltonian H_N^{MF}.

(A_1^{MF}) For $\alpha \in \{1,2\}$, the confining potentials satisfy $U_{\mathrm{trap}}^{(\alpha)} \in L^{3/2}_{\mathrm{loc}}(\mathbb{R}^3,\mathbb{R})$ and

$$U_{\mathrm{trap}}^{(\alpha)}(x) \to +\infty \quad \text{as} \quad |x| \to +\infty.$$

(A_2^{MF}) For $\alpha \in \{1,2,12\}$ the interaction potential $V^{(\alpha)} : \mathbb{R}^3 \to \mathbb{R}$ is measurable, spherically symmetric, and satisfies the inequality

$$\big(V^{(\alpha)}\big)^2 \;\leqslant\; C(\mathbb{1} - \Delta) \tag{3.2}$$

in the sense of forms. Moreover, we require the following Fourier point-wise inequalities to hold true:

$$\widehat{V^{(1)}} \geqslant 0\,, \qquad \widehat{V^{(2)}} \geqslant 0\,, \qquad \widehat{V^{(1)}}\widehat{V^{(2)}} \;\geqslant\; \big(\widehat{V^{(12)}}\big)^2. \tag{3.3}$$

Assumption (A_1^{MF}), already present in the GP setting in Chapter 2, ensures that the one-body operator $T^{(\alpha)} := -\Delta + U_{\mathrm{trap}}^{(\alpha)}$ is bounded from below, and with compact resolvent. The results presented below could be adapted to the case in which the Laplacian $-\Delta$ is replaced by the magnetic Laplacian $(i\nabla + A(x))^2$ or by the pseudo-relativistic Laplacian $\sqrt{-\Delta + m^2} - m$.

Condition (3.2) on the two-body potentials includes the case of a local Coulomb singularity $|x|^{-1}$.

Condition (3.3) is the non-local analogue of the miscibility condition (2.1), and will be explicitly used to prove the uniqueness of the minimum of the Hartree functional.

In order to define the Bogoliubov Hamiltonian, the second quantization formalism is needed. Let us introduce the single-component Fock spaces

$$\mathcal{F}^{(\alpha)} := \bigoplus_{n=0}^{\infty} \big(\mathfrak{h}^{(\alpha)}\big)^{\otimes_{\mathrm{sym}} n}, \qquad \mathfrak{h}^{(\alpha)} := L^2(\mathbb{R}^3), \qquad \alpha \in \{1,2\} \tag{3.4}$$

and the double-component Fock space

$$\mathcal{F} := \mathcal{F}^{(1)} \otimes \mathcal{F}^{(2)} = \bigoplus_{L=0}^{\infty} \Bigg(\bigoplus_{\substack{n,m\in\mathbb{N}_0 \\ n+m=L}} \big(\mathfrak{h}^{(1)}\big)^{\otimes_{\mathrm{sym}} n} \otimes \big(\mathfrak{h}^{(2)}\big)^{\otimes_{\mathrm{sym}} m} \Bigg). \tag{3.5}$$

Let $\{u_m\}_{m=0}^{\infty}$ and $\{v_n\}_{n=0}^{\infty}$ be orthonormal bases of $\mathfrak{h}^{(1)}$ and $\mathfrak{h}^{(2)}$, respectively, with (u_0, v_0) being the minimizer of the Hartree functional (1.17). We shall choose once and for all these two bases in such a way that all their elements belong to the domain of self-adjointness, respectively, of the operator $h^{(1)}$ on $\mathfrak{h}^{(1)}$ and of the operator $h^{(2)}$ on $\mathfrak{h}^{(2)}$ that we are going to define in formula (3.13) below. Let

$$a_m := a(u_m), \qquad a_m^* := a^*(u_m), \qquad b_n := b(v_n), \qquad b_n^* := b^*(v_n)\,. \tag{3.6}$$

be the usual creation and annihilation operators on $\mathcal{F}^{(1)}$ and $\mathcal{F}^{(2)}$, which are linear operators defined by the actions

$$\begin{aligned} (a_m\Psi_n)(x_1,\dots,x_{n-1}) &= \sqrt{n}\int_{\mathbb{R}^3} \mathrm{d}x\, \overline{u_m(x)}\, \Psi_n(x,x_1,\dots,x_{n-1}), \\ (a_m^*\Psi_n)(x_1,\dots,x_{n+1}) &= \frac{1}{\sqrt{n+1}} \sum_{j=1}^{n+1} u_m(x_j)\Psi_n(x_1,\dots,x_{j-1},x_j,\dots,x_{n+1}) \end{aligned} \tag{3.7}$$

for all $\Psi_n \in (\mathfrak{h}^{(1)})^{\otimes_{\mathrm{sym}} n}$ and for all $n \geqslant 0$, and similar actions for b_m, b_m^*. They satisfy the canonical commutation relations (CCR)

$$\begin{aligned} [a_m, a_n] &= 0 = [a_m^*, a_n^*], \qquad [a_m, a_n^*] = \delta_{m,n}\mathbb{1}_{\mathcal{F}_+^{(1)}}, \\ [b_m, b_n] &= 0 = [b_m^*, b_n^*]\,, \qquad [b_m, b_n^*] = \delta_{m,n}\mathbb{1}_{\mathcal{F}_+^{(2)}}. \end{aligned} \tag{3.8}$$

With no risk of confusion we shall keep denoting with a_m, a_m^*, b_m, b_m^* the operators

$$a_m \otimes \mathbb{1}_{\mathcal{F}^{(2)}}, \qquad a_m^* \otimes \mathbb{1}_{\mathcal{F}^{(2)}}, \qquad \mathbb{1}_{\mathcal{F}^{(1)}} \otimes b_m, \qquad \mathbb{1}_{\mathcal{F}^{(1)}} \otimes b_m^* \tag{3.9}$$

now acting on $\mathcal{F} = \mathcal{F}^{(1)} \otimes \mathcal{F}^{(2)}$. Obviously, a_m, a_m^* commute with b_n, b_n^*.

In terms of these operators, we can lift the N-body Hamiltonian H_N^{MF} on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ as an operator on the Fock space $\mathcal{F}$ as

$$\begin{aligned} H_N^{\mathrm{MF}} \;=\; & \sum_{m,n\geqslant 0} \Big(\langle u_m, (-\Delta + U^{(1)}_{\mathrm{trap}})u_n\rangle a^*_m a_n + \langle v_m, (-\Delta + U^{(2)}_{\mathrm{trap}})v_n\rangle b^*_m b_n \Big) \\ & + \frac{1}{N} \sum_{m,n,p,q} \Big(\tfrac12 V^{(1)}_{mnpq} a^*_m a^*_n a_p a_q + \tfrac12 V^{(2)}_{mnpq} b^*_m b^*_n b_p b_q + V^{(12)}_{mnpq} a^*_m b^*_n a_p b_q \Big) \end{aligned} \tag{3.10}$$

where

$$\begin{aligned} V^{(1)}_{mnpq} &:= \langle u_m, [V^{(1)} * (\overline{u_n} u_q)] u_p\rangle, \\ V^{(2)}_{mnpq} &:= \langle v_m, [V^{(2)} * (\overline{v_n} v_q)] v_p\rangle \\ V^{(12)}_{mnpq} &:= \langle u_m, [V^{(12)} * (\overline{v_n} v_q)] u_p\rangle. \end{aligned} \tag{3.11}$$

The scalar products in (3.11) are all finite due to the choice of the bases $\{u_m\}_{m=0}^\infty$ and $\{v_n\}_{n=0}^\infty$ and to (3.2).

Bogoliubov's approximation [13] suggests to formally replace a_0, a_0^* and b_0, b_0^* in (3.10) by the scalar values $\sqrt{N_1}$ and $\sqrt{N_2}$, respectively. This formal replacement would produce terms of order N, which sum up to Ne_{H} as in the r.h.s of (3.1), terms of order $\sqrt{N}$, of order 1, and sub-leading terms. The terms of order $\sqrt{N}$ are however canceled due to the Euler-Lagrange equations for the Hartree minimizer

$$h^{(1)} u_0 = 0, \quad h^{(2)} v_0 = 0, \tag{3.12}$$

where

$$\begin{aligned} h^{(1)} &:= -\Delta + U^{(1)}_{\mathrm{trap}} + c_1 V^{(1)} * |u_0|^2 + c_2 V^{(12)} * |v_0|^2 - \mu^{(1)} \\ h^{(2)} &:= -\Delta + U^{(2)}_{\mathrm{trap}} + c_2 V^{(2)} * |v_0|^2 + c_1 V^{(12)} * |u_0|^2 - \mu^{(2)}, \end{aligned} \tag{3.13}$$

and the chemical potentials are

$$\begin{aligned} \mu^{(1)} &:= \langle u_0, (-\Delta + U^{(1)}_{\mathrm{trap}}) u_0\rangle + c_1 \langle u_0, V^{(1)} * |u_0|^2 u_0\rangle + c_2 \langle u_0, V^{(12)} * |v_0|^2 u_0\rangle \\ \mu^{(2)} &:= \langle v_0, (-\Delta + U^{(2)}_{\mathrm{trap}}) v_0\rangle + c_2 \langle v_0, V^{(2)} * |v_0|^2 v_0\rangle + c_1 \langle u_0, V^{(12)} * |v_0|^2 u_0\rangle\,. \end{aligned} \tag{3.14}$$

Hence, by ignoring sub-leading contributions, Bogoliubov's approximation produces, besides the leading order term Ne_{H}, a series of N-independent terms which can be recast in the quadratic operator

$$\begin{aligned} \mathbb{H} := \sum_{m,n\geqslant 1} \Big[& \langle u_m, h^{(1)} u_n\rangle a^*_m\, a_n + \langle v_m, h^{(2)} v_n\rangle b^*_m\, b_n + c_1 V^{(1)}_{m00n} a^*_m a_n + c_2 V^{(2)}_{m00n} b^*_m b_n \\ & + \tfrac12\, c_2 V^{(2)}_{mn00} b^*_m b^*_n + \tfrac12\, c_2 \overline{V^{(2)}_{mn00}} b_m b_n + \tfrac12\, c_1 V^{(1)}_{mn00} a^*_m a^*_n + \tfrac12\, c_1 \overline{V^{(1)}_{mn00}} a_m a_n \\ & + \sqrt{c_1 c_2}\, V^{(12)}_{0mn0}\, b^*_m a_n + \sqrt{c_1 c_2}\, \overline{V^{(12)}_{0mn0}}\, a^*_m b_n \\ & + \sqrt{c_1 c_2}\, V^{(12)}_{mn00}\, a^*_m b^*_n + \sqrt{c_1 c_2}\, \overline{V^{(12)}_{mn00}}\, a_m b_n \Big] \\ & - \tfrac12\, c_1 V^{(1)}_{0000} - \tfrac12\, c_2 V^{(2)}_{0000} \end{aligned} \tag{3.15}$$

acting on the excited Fock space

$$\mathcal{F}_+ \;:=\; \mathcal{F}^{(1)}_+ \otimes \mathcal{F}^{(2)}_+ \;=\; \bigoplus_{L=0}^{\infty} \Bigg(\bigoplus_{\substack{n,m\in\mathbb{N}_0 \\ n+m=L}} \big(\mathfrak{h}^{(1)}_+\big)^{\otimes_{\mathrm{sym}} n} \otimes \big(\mathfrak{h}^{(2)}_+\big)^{\otimes_{\mathrm{sym}} m} \Bigg), \tag{3.16}$$

where

$$\mathfrak{h}_+^{(1)} := \{u_0\}^\perp \subset L^2(\mathbb{R}^3)\,, \qquad \mathfrak{h}_+^{(2)} := \{v_0\}^\perp \subset L^2(\mathbb{R}^3). \tag{3.17}$$

Note that $\mathbb{H}$ is independent of the choice of $\{u_m\}_{m=1}^\infty$ and $\{v_n\}_{n=1}^\infty$, apart from the technical assumption that these functions belong to the domains $\mathcal{D}(h^{(1)})$, $\mathcal{D}(h^{(2)})$ of the self-adjoint operators $h^{(1)}$, $h^{(2)}$, respectively. We can rigorously interpret $\mathbb{H}$ as a self-adjoint operator with core domain

$$\bigcup_{M=0}^{\infty} \bigoplus_{L=0}^{M} \Bigg(\bigoplus_{\substack{n,m\in\mathbb{N}_0 \\ n+m=L}} \big(\mathfrak{h}_+^{(1)} \cap D(h^{(1)})\big)^{\otimes_{\mathrm{sym}} n} \otimes \big(\mathfrak{h}_+^{(2)} \cap D(h^{(2)})\big)^{\otimes_{\mathrm{sym}} m} \Bigg). \tag{3.18}$$

The operator $\mathbb{H}$ is called *Bogoliubov Hamiltonian*. In Section 3.3 it will be characterized as the quantized form of (half) the Hessian of the Hartree functional evaluated on the minimizer.

We are now ready to state the main result of this Chapter.

Theorem 3.1 (Bogoliubov correction to the mean-field limit).
Let Assumptions (A_1^{MF}) and (A_2^{MF}) be satisfied. Then the following statements hold true.

(i) There exists a unique minimizer (u_0, v_0) (up to phases) for the variational problem

$$e_{\mathrm{H}} := \inf_{\substack{u,v\,\in\, H^1(\mathbb{R}^3) \\ \|u\|_2=\|v\|_2=1}} \mathcal{E}^{\mathrm{H}}[u,v].$$

(ii) The Bogoliubov Hamiltonian $\mathbb{H}$ in (3.15) *is bounded from below on $\mathcal{F}_+$ with core domain* (3.18). *Moreover, its self-adjoint realization, still denoted by $\mathbb{H}$, has a unique, non-degenerate ground state $\Phi^{\mathrm{gs}} = (\Phi^{\mathrm{gs}}_{m,n})_{m,n\geqslant 0} \in \mathcal{F}_+$.*

(iii) The ground state energy of H_N^{MF} satisfies

$$\lim_{N\to\infty} \big(E_N^{\mathrm{MF}} - N e_{\mathrm{H}}\big) \;=\; \inf \sigma(\mathbb{H})\,. \tag{3.19}$$

(iv) The ground state ψ_N^{gs} of H_N^{MF} satisfies the norm approximation

$$\lim_{N\to\infty} \Bigg\| \psi_N^{\mathrm{gs}} - \sum_{0\leqslant m\leqslant N_1} \sum_{0\leqslant n\leqslant N_2} \frac{(a_0^*)^{N_1-m}}{\sqrt{(N_1-m)!}} \frac{(b_0^*)^{N_2-n}}{\sqrt{(N_2-n)!}} \Phi^{\mathrm{gs}}_{m,n} \Bigg\|_{\mathcal{H}_{N_1,N_2,\mathrm{sym}}} = 0. \tag{3.20}$$

up to an overall phase factor for Φ^{gs} that does not depend on $m, n, N_1,$ or N_2.

We remark that the ground state ψ_N^{gs} of H_N^{MF} is unique, up to complex phases. More precisely, in case of no magnetic fields (as in Theorem 3.1), the ground state of H_N^{MF} under the partial symmetry conditions of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ coincides with the ground state in absence of symmetry (see [54, Section 3.2.4]). Hence, uniqueness and pointwise positivity of ψ_N^{gs} follow from standard properties of Schrödinger operators (see e.g. [51, Chapter 11]). It is to be remarked that a result similar to Theorem 3.1 holds for the excitation spectrum of H_N^{MF}, but we focus on the ground state only in order to simplify the presentation.

In the one-component case, Bogoliubov's second order correction for the ground state energy and the excitation spectrum in the mean-field regime were obtained first by Seiringer [88] for the homogeneous Bose gas (i.e. for particles confined on a unit torus and without external potentials), and by Grech and Seiringer [35] for the non-homogeneous trapped gas. Then Lewin, Nam, Serfaty, and Solovej [49] introduced a different approach which covers very general assumptions and in particular Coulomb-type potentials. Further extensions include a mixed mean-field large-volume limit by Dereziński and Napiorkówski [25], collective excitations and multiple condensations by Nam and Seiringer [75], N^{-1}-power expansion formulas by Pizzo [85], and an infinitely-splitting double-well model by Rougerie and Spehner [86]. In the very recent work [11], Boccato, Brennecke, Cenatiempo, and Schlein were able to justify Bogoliubov's theory in the Gross-Pitaevskii limit for the homogeneous Bose gas. We expect a similar result to hold for the multi-component case as well.

We will prove Theorem 3.1 in the remaining part of this Chapter. More precisely, (i) will be proved in Section 3.2, (ii) in Section 3.3, while (iii) and (iv) in Section 3.5. For the proof of (iii) and (iv) we will follow the general strategy of the work [49] and add suitable adaptations in order to take into account the two-component structure.

3.2 Leading order and uniqueness of the Hartree minimizer

Let us start with discussing the mean-field analogue of Theorem (2.1).

Theorem 3.2 (Leading order in the mean-field limit).
Let Assumptions (A_1^{MF}) and (A_2^{MF}) be satisfied.

(I) There exists a unique minimizer (u_0, v_0) (up to phases) for the variational problem

$$e_{\mathrm{H}} \ := \inf_{\substack{u,v\,\in\, H^1(\mathbb{R}^3) \\ \|u\|_{L^2}=\|v\|_{L^2}=1}} \mathcal{E}^{\mathrm{H}}[u,v].$$

(II) The ground state energy of H_N^{MF} satisfies

$$\lim_{N\to\infty} \frac{E_N^{\mathrm{MF}}}{N} \ = \ e_{\mathrm{H}}. \tag{3.21}$$

(III) If ψ_N is an approximate ground state of H_N^{MF}, in the sense that

$$\lim_{N\to\infty} \frac{\langle \psi_N, H_N^{\mathrm{MF}} \psi_N\rangle}{N} \ = \ e_{\mathrm{H}},$$

then it exhibits complete double-component Bose-Einstein condensation:

$$\lim_{N\to+\infty} \gamma_{\psi_N}^{(k,\ell)} \ = \ |u_0^{\otimes k}\otimes v_0^{\otimes \ell}\rangle\langle u_0^{\otimes k}\otimes v_0^{\otimes \ell}|, \quad \forall k,\ell = 0,1,2,... \tag{3.22}$$

in trace class.

As was the case for Theorem 2.1, Theorem 3.2 justifies the assumptions on the initial states for the analysis of the time evolution generated by H_N^{MF} that will be presented in Chapter 4. There one proves that double-component condensation is preserved by time evolution as soon as it holds for the initial datum, and Theorem 3.2 provides a physically relevant and preparable class of initial data.

We will prove Theorem 3.2 in the remaining part of this Section. In doing so, we will provide the proof of Theorem 3.1 (i), since this coincides with Theorem 3.2 (I).

Proof. The proof of Theorem 3.2 is similar to (and to some extent easier than) the proof of Theorem 2.1. Let us briefly explain the necessary adaptations.

Part (I). The existence of minimizers of e_{H} is standard. The uniqueness of the minimizer (up to complex phases) is based on a convexity argument. More precisely, if we define $\mathcal{D}^{\mathrm{H}}[f,g] := \mathcal{E}^{\mathrm{H}}[\sqrt{f},\sqrt{g}]$ for $f,g \geqslant 0$, then $\mathcal{D}^{\mathrm{H}}$ is convex. Indeed, by considering $\mathcal{D}^{\mathrm{H}}_1$, $\mathcal{D}^{\mathrm{H}}_2$ and $\mathcal{D}^{\mathrm{H}}_{12}$ as the summands of the Hartree functional containing respectively $V^{(1)}$, $V^{(2)}$ and $V^{(12)}$, we obtain the following identities

$$\begin{aligned}
\frac{\mathcal{D}^{\mathrm{H}}_1[f,g]+\mathcal{D}^{\mathrm{H}}_1[r,s]}{2} - \mathcal{D}^{\mathrm{H}}_1\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] &= \frac{c_1^2}{2}\int \mathrm{d}k\,\Big|\frac{\widehat{f}(k)-\widehat{r}(k)}{2}\Big|^2\widehat{V^{(1)}}(k),\\
\frac{\mathcal{D}^{\mathrm{H}}_2[f,g]+\mathcal{D}^{\mathrm{H}}_2[r,s]}{2} - \mathcal{D}^{\mathrm{H}}_2\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] &= \frac{c_2^2}{2}\int \mathrm{d}k\,\Big|\frac{\widehat{g}(k)-\widehat{s}(k)}{2}\Big|^2\widehat{V^{(2)}}(k),\\
\frac{\mathcal{D}^{\mathrm{H}}_{12}[f,g]+\mathcal{D}^{\mathrm{H}}_{12}[r,s]}{2} - \mathcal{D}^{\mathrm{H}}_{12}\Big[\frac{f+r}{2},\frac{g+s}{2}\Big] &= c_1c_2\int \mathrm{d}k\,\overline{\frac{\widehat{f}(k)-\widehat{r}(k)}{2}}\,\frac{\widehat{g}(k)-\widehat{s}(k)}{2}\,\widehat{V^{(12)}}(k).
\end{aligned}$$

Therefore, the convexity follows from the Cauchy-Schwarz inequality and Assumption (3.3).

From now on the proof follows the same steps as the proof of part (i) of Theorem 2.1, and hence we omit it.

Part (II) and (III). The energy upper bound

$$\limsup_{N\to\infty}\frac{E^{\mathrm{MF}}_N}{N} \leqslant e_{\mathrm{H}} \tag{3.23}$$

follows easily by choosing the trial state $u^{\otimes N_1}\otimes v^{\otimes N_2}$.

To prove the lower bound for (II) and to prove (III) we adapt to the two-component case the methods used in [47].

Let $\psi_N \in \mathcal{H}_{N_1,N_2,\mathrm{sym}}$ satisfy

$$\langle \psi_N, H^{\mathrm{MF}}_N\psi_N\rangle \leqslant E^{\mathrm{MF}}_N + o(N). \tag{3.24}$$

Using the upper bound and the definition of reduced density matrices (1.3) we write

$$\begin{aligned}
e_{\mathrm{H}}+o(1)_{N\to\infty} \geqslant \frac{\langle\psi_N, H^{\mathrm{MF}}_N\psi_N\rangle}{N} &= c_1\,\mathrm{Tr}\Big[T^{(1)}\gamma^{(1,0)}_{\psi_N}\Big] + \frac{c_1^2}{2}\,\mathrm{Tr}\Big[V^{(1)}(x_1-x_2)\gamma^{(2,0)}_{\psi_N}\Big]\\
&\quad + c_2\,\mathrm{Tr}\Big[T^{(2)}\gamma^{(0,1)}_{\psi_N}\Big] + \frac{c_2^2}{2}\,\mathrm{Tr}\Big[V^{(2)}(y_1-y_2)\gamma^{(0,2)}_{\psi_N}\Big]\\
&\quad + c_1c_2\,\mathrm{Tr}\Big[V^{(12)}(x-y)\gamma^{(1,1)}_{\psi_N}\Big],
\end{aligned} \tag{3.25}$$

where $T^{(\alpha)} := -\Delta + U^{(\alpha)}_{\mathrm{trap}}$. Using assumptions (A^{MF}_1) and (A^{MF}_2) we obtain the operator inequalities

$$\pm V^{(1)}(x_1-x_2) \leqslant \varepsilon T^{(1)}_{x_1} + C_\varepsilon, \tag{3.26}$$

$$\pm V^{(2)}(y_1-y_2) \leqslant \varepsilon T^{(2)}_{y_1} + C_\varepsilon, \tag{3.27}$$

$$\pm V^{(12)}(x-y) \leqslant \varepsilon (T^{(1)}_{x} + T^{(2)}_{y}) + C_\varepsilon \tag{3.28}$$

for all $\varepsilon > 0$.

Last estimates combined with (3.25) imply that $\mathrm{Tr}[T^{(1)}\gamma^{(1,0)}_{\psi_N}]$ and $\mathrm{Tr}[T^{(2)}\gamma^{(0,1)}_{\psi_N}]$ are bounded uniformly in N. Since $T^{(1)}$ and $T^{(2)}$ have compact resolvent, up to a subsequence as $N\to\infty$, $\gamma^{(1,0)}_{\psi_N}$ and $\gamma^{(0,1)}_{\psi_N}$ converge strongly in trace class. Thus, the Quantum de Finetti Theorem 1.3 ensures that, up to a subsequence again, there exists a Borel probability measure μ supported on the set

$$\{(u,v) : u,v\in L^2(\mathbb{R}^3), \|u\|=\|v\|=1\}$$

such that

$$\lim_{N\to\infty}\gamma^{(k,\ell)}_{\psi_N} \;=\; \int |u^{\otimes k}\otimes v^{\otimes \ell}\rangle\langle u^{\otimes k}\otimes v^{\otimes\ell}|\,\mathrm{d}\mu(u,v),\quad \forall k,\ell=0,1,2,\ldots \tag{3.29}$$

strongly in trace class.

Next, the operator inequality (3.26) implies

$$\frac{c_1}{4}T^{(1)}_{x_1}+\frac{c_1}{4}T^{(1)}_{x_2}+\frac{c_1^2}{2}V^{(1)}(x_1-x_2)\;\geqslant\;-C.$$

Therefore, from the convergence (3.29) and Fatou's lemma, it follows that

$$\begin{aligned}
&\liminf_{N\to\infty}\mathrm{Tr}\Big[\Big(\frac{c_1}{4}T^{(1)}_{x_1}+\frac{c_1}{4}T^{(1)}_{x_2}+\frac{c_1^2}{2}V^{(1)}(x_1-x_2)\Big)\gamma^{(2,0)}_{\psi_N}\Big]\\
&\qquad\geqslant\;\mathrm{Tr}\Big[\Big(\frac{c_1}{4}T^{(1)}_{x_1}+\frac{c_1}{4}T^{(1)}_{x_2}+\frac{c_1^2}{2}V^{(1)}(x_1-x_2)\Big)\int|u^{\otimes 2}\rangle\langle u^{\otimes 2}|\,\mathrm{d}\mu(u,v)\Big]\\
&\qquad=\;\int\Big[\frac{c_1}{2}\langle u,T^{(1)}u\rangle+\frac{c_1^2}{2}\langle|u|^2,V^{(1)}*|u|^2\rangle\Big]\,\mathrm{d}\mu(u,v).
\end{aligned}$$

Similarly, we have

$$\begin{aligned}
&\liminf_{N\to\infty}\mathrm{Tr}\Big[\Big(\frac{c_1}{4}T^{(2)}_{y_1}+\frac{c_2}{4}T^{(2)}_{y_2}+\frac{c_2^2}{2}V^{(2)}(y_1-y_2)\Big)\gamma^{(0,2)}_{\psi_N}\Big]\\
&\qquad\geqslant\;\int\Big[\frac{c_2}{2}\langle v,T^{(2)}v\rangle+\frac{c_2^2}{2}\langle|v|^2,V^{(2)}*|v|^2\rangle\Big]\mathrm{d}\mu(u,v)
\end{aligned}$$

and

$$\begin{aligned}
&\liminf_{N\to\infty}\mathrm{Tr}\Big[\Big(\frac{c_1}{2}T^{(1)}_{x}+\frac{c_2}{2}T^{(2)}_{y}+c_1c_2V^{(12)}(x-y)\Big)\gamma^{(1,1)}_{\psi_N}\Big]\\
&\qquad\geqslant\int\Big[\frac{c_1}{2}\langle u,T^{(1)}u\rangle+\frac{c_2}{2}\langle v,T^{(2)}v\rangle+c_1c_2\langle uv,V^{(12)}*(uv)\rangle\Big]\,\mathrm{d}\mu(u,v).
\end{aligned}$$

Summing these lower bounds, we can continue to the right the chain of inequalities (3.25), so as to obtain

$$\liminf_{N\to\infty}\frac{\langle\psi_N,H_N\psi_N\rangle}{N}\;\geqslant\;\int\mathcal{E}_{\mathrm{H}}[u,v]\,\mathrm{d}\mu(u,v)\;\geqslant\;e_{\mathrm{H}}.$$

Combining last estimate with the upper bound (3.23), we obtain (3.21):

$$\lim_{N\to\infty}\frac{\langle\psi_N,H_N\psi_N\rangle}{N}\;=\;\int\mathcal{E}_{\mathrm{H}}[u,v]\,\mathrm{d}\mu(u,v)\;=\;e_{\mathrm{H}}.$$

Last equality means that μ is supported on the set of Hartree minimizers, i.e., $\{(e^{i\theta_1}u_0,e^{i\theta_2}v_0):\theta_1,\theta_2\in\mathbb{R}\}$, hence (3.29) reduces to (3.22). Strictly speaking, we have proved (3.21) and (3.22) for a subsequence as $N\to\infty$, but the convergence must hold for the whole sequence because the limits are unique. This completes the proof. $\square$

3.3 Qualification of the Bogoliubov Hamiltonian

The aim of this Section is to show that the Bogoliubov Hamiltonian $\mathbb{H}$ defined in (3.15) is precisely the same operator that arises from a suitable second quantization of the Hessian of the Hartree functional $\mathcal{E}^{\mathrm{H}}$ evaluated at the minimizer (u_0, v_0). In doing so we will also prove (*ii*) of Theorem 3.1. To this aim, it is useful to recall the explicit (canonical) isomorphism that realizes $\mathcal{F}_+$ in (3.16) as a Fock space.

We consider the Fock space with base space $\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$

$$\mathcal{G}_+ := \bigoplus_{N=0}^{\infty} \big(\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}\big)^{\otimes_{\mathrm{sym}} N}. \tag{3.30}$$

For a generic $f \oplus g \in \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$, let us denote the canonical creation and annihilation operators on $\mathcal{G}_+$ as $Z^*(f \oplus g), Z(f \oplus g)$. The N-th sector of $\mathcal{G}_+$ is interpreted as the space of states with *exactly* N total particles, regardless of which type they are. In fact (see, e.g. [24, Theorems 16 and 19]) $\mathcal{G}_+$ is isomorphic to $\mathcal{F}_+$ through a natural isomorphism that preserves the CCR.

Theorem 3.3. *There exists a unitary operator $U : \mathcal{F}_+ \to \mathcal{G}_+$ such that*

(i) $U(\Omega_{\mathcal{F}_+}) = \Omega_{\mathcal{G}_+}$, where $\Omega_{\mathcal{F}_+}$ is the vacuum of $\mathcal{F}_+$ and $\Omega_{\mathcal{G}_+}$ is the vacuum of $\mathcal{G}_+$,

(ii) for any $f \oplus g \in \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$

$$\begin{aligned} Z^*(f \oplus g)U &= U\big(a^*(f) \otimes \mathbb{1} + \mathbb{1} \otimes b^*(g)\big) \\ Z(f \oplus g)U &= U\big(a(f) \otimes \mathbb{1} + \mathbb{1} \otimes b(g)\big). \end{aligned}$$

We define the second quantization of a self-adjoint operator $\mathcal{A}$ on $\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$ by

$$\mathrm{d}\Gamma(\mathcal{A}) := \sum_{m,n \geqslant 1} \langle f_m, \mathcal{A} f_n \rangle Z^*(f_m) Z(f_n), \tag{3.31}$$

where $\{f_m\}_{m=1}^{\infty}$ is an orthonormal basis of $\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$ belonging entirely to the domain of $\mathcal{A}$, with an overall *operator closure* being understood on the right side. Similarly, for generic self-adjoint operators $A^{(1)}$ on $\mathfrak{h}_+^{(1)}$ and $A^{(2)}$ on $\mathfrak{h}_+^{(2)}$, we denote

$$\begin{aligned} \mathrm{d}\Gamma^{(1)}(A^{(1)}) \;&:=\; \sum_{m,n \geqslant 1} \langle u_m, A^{(1)} u_n \rangle a_m^* a_n \\ \mathrm{d}\Gamma^{(2)}(A^{(2)}) \;&:=\; \sum_{m,n \geqslant 1} \langle v_m, A^{(2)} v_n \rangle b_m^* b_n \,, \end{aligned} \tag{3.32}$$

with $\{u_m\}_{m=1}^{\infty}$ an orthonormal basis of $\mathfrak{h}_+^{(1)}$ and $\{v_n\}_{n=1}^{\infty}$ an orthonormal basis of $\mathfrak{h}_+^{(2)}$. In particular,

$$\mathcal{N}_1 \;:=\; \mathrm{d}\Gamma^{(1)}(\mathbb{1})\,, \qquad \mathcal{N}_2 \;:=\; \mathrm{d}\Gamma^{(2)}(\mathbb{1}) \tag{3.33}$$

defines the number operators in each species' sectors, and

$$\mathcal{N} \;:=\; \mathcal{N}_1 + \mathcal{N}_2 \tag{3.34}$$

defines the total number operator on $\mathcal{F}_+$.

Within this formalism, it is natural to introduce the class of quadratic Hamiltonians in the Fock space $\mathcal{G}_+$; through the isomorphism of Theorem 3.3, such a class turns out to correspond to the class of Hamiltonians which are *jointly* quadratic in a, a^*, b, and b^*, as is the case for $\mathbb{H}$. Note that, already the operators defined by (3.31), which are quadratic in Z and Z^*, are in general not separately quadratic in a, a^* or b, b^*; this is true only if the operator $\mathcal{A}$ is reduced with respect to the direct sum $\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$.

Let us consider two densely defined operators

$$\begin{aligned} \mathcal{B}_1 &: \mathcal{D}(\mathcal{B}_1) \subset \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)} \to \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)} \\ \mathcal{B}_2 &: \mathcal{D}(\mathcal{B}_2) \subset \big(\mathfrak{h}_+^{(1)}\big)^* \oplus \big(\mathfrak{h}_+^{(2)}\big)^* \to \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)} \end{aligned}$$

satisfying the properties

$$\mathcal{D}(\mathcal{B}_1) \subset J^*\mathcal{D}(\mathcal{B}_2), \quad \mathcal{B}_1^* \;=\; \mathcal{B}_1, \quad J\mathcal{B}_2 J \;=\; \mathcal{B}_2^*,$$

where

$$J : \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)} \to \big(\mathfrak{h}_+^{(1)}\big)^* \oplus \big(\mathfrak{h}_+^{(2)}\big)^*, \qquad J(f \oplus g) := \langle f \oplus g, \cdot\, \rangle_{\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}} \tag{3.35}$$

is the operator mapping a vector to the corresponding form. Let us form the operator

$$\mathcal{B} \;:=\; \begin{pmatrix} \mathcal{B}_1 & \mathcal{B}_2 \\ \mathcal{B}_2^* & J\mathcal{B}_1 J^* \end{pmatrix} \tag{3.36}$$

acting on the space

$$\mathfrak{h} \;:=\; \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)} \oplus \big(\mathfrak{h}_+^{(1)}\big)^* \oplus \big(\mathfrak{h}_+^{(2)}\big)^*. \tag{3.37}$$

We define

$$\mathbb{H}_{\mathcal{B}} \;:=\; \mathrm{d}\Gamma(\mathcal{B}_1) + \frac{1}{2}\sum_{m,n\geqslant 1}\Big(\langle f_m, \mathcal{B}_2 J f_n\rangle Z(f_m)Z(f_n) + \overline{\langle f_m, \mathcal{B}_2 J f_n\rangle} Z^*(f_m)Z^*(f_n)\Big) \tag{3.38}$$

on the space

$$\bigoplus_{n=0}^{\infty} \mathcal{D}(\mathcal{B}_1)^{\otimes_{\mathrm{sym}} n}.$$

In turns out that several properties of the quadratic Hamiltonian $\mathbb{H}_{\mathcal{B}}$ depend crucially on those of the corresponding classical operator $\mathcal{B}$. The following Lemma, which is a consequence of [73, Theorem 2], collects some of them.

Lemma 3.4. *Assume that $\mathcal{B}_1 > 0$, $\mathcal{B} > 0$ and that $\mathcal{B}_2$ is a Hilbert-Schmidt operator. Assume further that $\|\mathcal{B}_1^{-1/2}\mathcal{B}_2 J\mathcal{B}_1^{-1/2}\| < 1$. Then:*

(i) (Self-adjointness) Formula (3.38) defines a self-adjoint operator.

(ii) (Uniqueness of the ground state) $\mathbb{H}_{\mathcal{B}}$ has a unique ground state $\Phi_{\mathcal{B}}^{\mathrm{gs}}$.

(iii) (Spectral gap) If, in addition, $\mathcal{B} \geqslant \tau > 0$ for some $\tau > 0$, then

$$\inf \sigma(\mathbb{H}_{|\{\Phi_{\mathcal{B}}^{\mathrm{gs}}\}^\perp}) \;>\; \lambda(\mathbb{H}_{\mathcal{B}}), \tag{3.39}$$

where $\lambda(\mathbb{H}_{\mathcal{B}})$ is the ground state energy of $\mathbb{H}_{\mathcal{B}}$.

In particular, $\mathbb{H}_{\mathcal{B}}$ is bounded from below, namely there exists a constant $C_{\mathcal{B}} > 0$ such that

$$\mathbb{H}_{\mathcal{B}} \;\geqslant\; -C_{\mathcal{B}}. \tag{3.40}$$

Proof. All the claims follow directly from Theorem 2 in [73]: by such result there exists a unitary operator $\mathbb{U}$ on $\mathcal{G}_+$ such that

$$\mathbb{U}\mathbb{H}_{\mathcal{B}}\mathbb{U}^* \;=\; \mathrm{d}\Gamma(\xi) + \inf\sigma(\mathbb{H}_{\mathcal{B}}), \tag{3.41}$$

for a positive operator ξ on $\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$. This proves the self-adjointness and implies that $\mathbb{U}\Omega_{\mathcal{G}_+}$ is the unique ground state of $\mathbb{H}_{\mathcal{B}}$. If, in addition, $\mathcal{B} \geqslant \tau > 0$, then $\xi \geqslant \tau > 0$, and this implies (3.39). $\square$

Notice that in Lemma 3.4 we require $\mathcal{B}_2$ to be Hilbert-Schmidt, an assumption which is fulfilled in the application we are interested in, and which ensures the weaker hypotheses in [73] to be satisfied.

Our interest in operators of the form $\mathbb{H}_{\mathcal{B}}$ is due to the fact that the Bogoliubov Hamiltonian (3.15) can be realized as a quadratic Hamiltonian in the sense of (3.38). More precisely,

$$\mathbb{H} \;=\; U^* \mathbb{H}_{\mathrm{Hess}\,\mathcal{E}^{\mathrm{H}}[u_0,v_0]} U, \tag{3.42}$$

where $\mathrm{Hess}\,\mathcal{E}^{\mathrm{H}}[u_0,v_0]$ is the Hessian of the Hartree functional evaluated at the minimizer and U is given by Theorem 3.3. In the present context the Hessian of the Hartree functional is defined by the second term of a Taylor expansion around the minimizer (u_0, v_0), that is,

$$\begin{aligned}\mathcal{E}^{\mathrm{H}}[u,v] \;&=\; \mathcal{E}^{\mathrm{H}}[u_0,v_0] \\ &\quad + \frac{1}{2}\big\langle \sqrt{c_1}(u-u_0) \oplus \sqrt{c_2}(v-v_0), \mathrm{Hess}\,\mathcal{E}^{\mathrm{H}}[u_0,v_0]\sqrt{c_1}(u-u_0) \oplus \sqrt{c_2}(v-v_0)\big\rangle \\ &\quad + o\big(\|u-u_0\|, \|v-v_0\|\big).\end{aligned} \tag{3.43}$$

In (3.43) we are considering variations that are *weighted* according to the relative populations of the two species.

In order to explicitly write the expression of $\mathrm{Hess}\,\mathcal{E}^{\mathrm{H}}[u_0,v_0]$, let us introduce the following three integral operators $K^{(\alpha)}$, $\alpha \in \{1,2,12\}$, together with their kernels:

$$K^{(1)} : \mathfrak{h}_+^{(1)} \to \mathfrak{h}^{(1)}, \qquad K^{(1)}(x,y) \;:=\; V^{(1)}(x-y)u_0(x)u_0(y) \tag{3.44}$$

$$K^{(2)} : \mathfrak{h}_+^{(2)} \to \mathfrak{h}^{(2)}, \qquad K^{(2)}(x,y) \;:=\; V^{(2)}(x-y)v_0(x)v_0(y) \tag{3.45}$$

$$K^{(12)} : \mathfrak{h}_+^{(2)} \to \mathfrak{h}^{(1)}, \qquad K^{(12)}(x,y) \;:=\; V^{(12)}(x-y)u_0(x)v_0(y). \tag{3.46}$$

With the quantities introduced in (3.11) we can write

$$\begin{aligned}\langle u_m, K^{(1)} u_n\rangle \;&=\; V^{(1)}_{m00n} \qquad & \langle u_m, K^{(1)}\overline{u_n}\rangle \;&=\; V^{(1)}_{mn00} \\ \langle v_m, K^{(2)} v_n\rangle \;&=\; V^{(2)}_{m00n} \qquad & \langle v_m, K^{(2)}\overline{v_n}\rangle \;&=\; V^{(2)}_{mn00} \\ \langle u_m, K^{(12)} v_n\rangle \;&=\; V^{(12)}_{m00n} \qquad & \langle u_m, K^{(12)}\overline{v_n}\rangle \;&=\; V^{(12)}_{mn00}.\end{aligned}$$

Moreover, as a straightforward consequence of Assumption (A_2^{MF}), each such operator is Hilbert-Schmidt: indeed,

$$\|K^{(1)}\|^2_{\mathrm{HS}} \;=\; \int \mathrm{d}x\mathrm{d}y |K^{(1)}(x,y)|^2 \leqslant C^{(1)} + C^{(1)}\|\nabla u_0\|_2^2 + C^{(1)}\|\nabla v_0\|_2^2 < +\infty, \tag{3.47}$$

and the same holds for $K^{(2)}$ and $K^{(12)}$.

In terms of the K's, and of $h^{(1)}$ and $h^{(2)}$ defined in (3.13), the Hessian of the Hartree functional reads

$$\begin{aligned}&\operatorname{Hess}\mathcal{E}^{\mathrm{H}}[u_0,v_0] \;=\\ &\begin{pmatrix} h^{(1)}+c_1K^{(1)} & \sqrt{c_1c_2}K^{(12)} & c_1K^{(1)}J^* & \sqrt{c_1c_2}K^{(12)}J^* \\ \sqrt{c_1c_2}K^{(12)*} & h^{(2)}+c_2K^{(2)} & \sqrt{c_1c_2}K^{(12)*}J^* & c_2K_2^{(2)}J^* \\ c_1JK^{(1)} & \sqrt{c_1c_2}JK^{(12)} & Jh^{(1)}J^*+c_1JK^{(1)}J^* & \sqrt{c_1c_2}JK_1^{(12)}J^* \\ \sqrt{c_1c_2}JK^{(12)*} & c_2JK^{(2)} & \sqrt{c_1c_2}JK^{(12)*}J^* & Jh^{(2)}J^*+c_2JK^{(2)}J^*\end{pmatrix}\end{aligned} \tag{3.48}$$

as a matrix-valued operator acting on $\mathfrak{h}_+^{(1)}\oplus\mathfrak{h}_+^{(2)}\oplus\big(\mathfrak{h}_+^{(1)}\big)^*\oplus\big(\mathfrak{h}_+^{(2)}\big)^*$.

The main result of this Section is the following

Theorem 3.5 (Bounds on Bogoliubov Hamiltonian)**.** *Under the same hypotheses of Theorem 3.1, one has*

$$\begin{aligned}\frac{1}{C}\big(\mathrm{d}\Gamma^{(1)}(h^{(1)})+\mathrm{d}\Gamma^{(2)}(h^{(2)})+\mathcal{N}_1+\mathcal{N}_2\big)-C \;&\leqslant\; \mathbb{H}\\ &\leqslant\; \mathrm{d}\Gamma^{(1)}(h^{(1)})+\mathrm{d}\Gamma^{(2)}(h^{(2)})+C\mathcal{N}_1+C\mathcal{N}_2+C,\end{aligned} \tag{3.49}$$

for some constant $C>0$. Consequently, $\mathbb{H}$ has a self-adjoint (Friedrichs) extension, still denoted by $\mathbb{H}$, with the same form domain of $\mathrm{d}\Gamma^{(1)}(h^{(1)}+1)+\mathrm{d}\Gamma^{(2)}(h^{(2)}+1)$*. Moreover, $\mathbb{H}$ has a unique, non-degenerate ground state Φ^{gs}:*

$$\inf\sigma(\mathbb{H}_{|\{\Phi^{\mathrm{gs}}\}^\perp}) \;>\; \langle\Phi^{\mathrm{gs}},\mathbb{H}\Phi^{\mathrm{gs}}\rangle. \tag{3.50}$$

Theorem 3.5 directly implies (ii) of Theorem 3.1.

As a preparatory result towards the proof of Theorem 3.5, we show that $\operatorname{Hess}\mathcal{E}^{\mathrm{H}}[u_0,v_0]$ has a strictly positive bottom.

Lemma 3.6. *There exists a constant $\eta>0$ such that*

$$\operatorname{Hess}\mathcal{E}^{\mathrm{H}}[u_0,v_0] \;\geqslant\; \eta. \tag{3.51}$$

This is clearly a non-degeneracy result for the minimizer (u_0,v_0) of the Hartree functional.

Proof. We consider the decomposition

$$\operatorname{Hess}\mathcal{E}^{\mathrm{H}}[u_0,v_0] \;=\; \operatorname{Hess}_h+\operatorname{Hess}_K,$$

where

$$\begin{aligned}\operatorname{Hess}_h \;&:=\; \begin{pmatrix} h^{(1)} & 0 & 0 & 0 \\ 0 & h^{(2)} & 0 & 0 \\ 0 & 0 & Jh^{(1)}J^* & 0 \\ 0 & 0 & 0 & Jh^{(2)}J^*\end{pmatrix}\\ \operatorname{Hess}_K \;&:=\; \begin{pmatrix} c_1K^{(1)} & \sqrt{c_1c_2}K^{(12)} & c_1K^{(1)}J^* & \sqrt{c_1c_2}K^{(12)}J^* \\ \sqrt{c_1c_2}K^{(12)*} & c_2K^{(2)} & \sqrt{c_1c_2}K^{(12)*}J^* & c_2K^{(2)}J^* \\ c_1JK^{(1)} & \sqrt{c_1c_2}JK^{(12)} & c_1JK^{(1)}J^* & \sqrt{c_1c_2}JK^{(12)}J^* \\ \sqrt{c_1c_2}JK^{(12)*} & c_2JK^{(2)} & \sqrt{c_1c_2}JK^{(12)*}J^* & c_2JK^{(2)}J^*\end{pmatrix}.\end{aligned} \tag{3.52}$$

First, we argue that Hess_h must be bounded away from zero. Indeed, since (u_0, v_0) is the unique minimizer of the Hartree functional, one has $h^{(1)} > 0$ on $\mathfrak{h}_+^{(1)}$ and $h^{(2)} > 0$ on $\mathfrak{h}_+^{(2)}$. Since Assumptions (A_1^{MF}) and (A_2^{MF}) imply that $h^{(1)}$ and $h^{(2)}$ have compact resolvent, their spectra cannot accumulate to zero, and this implies the existence of some $\eta > 0$ such that

$$\mathrm{Hess}_h \;\geqslant\; \eta. \tag{3.53}$$

Concerning Hess_K, we observe that it is a matrix-valued operator with structure

$$\mathrm{Hess}_K \;=\; \begin{pmatrix} \mathcal{A} & \mathcal{A}J^* \\ J\mathcal{A} & J\mathcal{A}J \end{pmatrix}$$

where

$$\mathcal{A} \;:=\; \begin{pmatrix} c_1 K^{(1)} & \sqrt{c_1 c_2} K^{(12)} \\ \sqrt{c_1 c_2} K^{(12)} & c_2 K^{(2)} \end{pmatrix}. \tag{3.54}$$

Since for any $f \oplus g \in \mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$ one has

$$\langle f \oplus g, \mathcal{A}\, f \oplus g \rangle \;=\; c_1 \langle f, K^{(1)} f \rangle + c_2 \langle g, K^{(2)} g \rangle + 2\sqrt{c_1 c_2}\, \mathbb{R}e\, \langle f, K^{(12)} g \rangle,$$

it is straightforward to see that, by Cauchy-Schwarz, Assumption (A_2^{MF}) implies $\mathcal{A} \geqslant 0$. Hence, $\mathrm{Hess}_K \geqslant 0$ follows. This result, together with (3.53), implies $\mathrm{Hess}\, \mathcal{E}^{\mathrm{H}}[u_0, v_0] \geqslant \eta > 0$. □

We can finally prove Theorem 3.5.

Proof of Theorem 3.5. We recognize that $\mathbb{H} = U^* \mathbb{H}_{\mathcal{B}} U$ with $\mathcal{B} = \mathrm{Hess}\, \mathcal{E}^{\mathrm{H}}[u_0, v_0]$, and, comparing (3.48) with (3.36), we deduce that

$$\mathcal{B}_2 \;=\; \begin{pmatrix} c_1 K^{(1)} J^* & \sqrt{c_1 c_2} K^{(12)} J^* \\ \sqrt{c_1 c_2} K^{(12)*} J^* & c_2 K^{(2)} J^* \end{pmatrix} \tag{3.55}$$

and

$$\mathcal{B}_1 \;=\; \begin{pmatrix} h^{(1)} & 0 \\ 0 & h^{(2)} \end{pmatrix} + \mathcal{B}_2 J.$$

Since $\mathcal{B}_1 > 0$, $\mathrm{Hess}\, \mathcal{E}^{\mathrm{H}}[u_0, v_0] > 0$ by Lemma 3.6, $\mathcal{B}_2$ is Hilbert-Schmidt, and $\|\mathcal{B}_1^{-1/2} \mathcal{B}_2 J \mathcal{B}_1^{-1/2}\| < 1$, we can apply Lemma 3.4. As a direct consequence we have that $\mathbb{H}$ is bounded from below.

We now show that the argument can be re-done so as to get the more refined lower bound (3.49). Indeed, it is easy to see that, for $\varepsilon > 0$ small enough, the operator

$$\begin{aligned} \mathcal{B}_\varepsilon \;:=\; & \mathrm{Hess}\, \mathcal{E}^{\mathrm{H}}[u_0, v_0] \\ & - \varepsilon \begin{pmatrix} h^{(1)} + \mathbb{1} & 0 & 0 & 0 \\ 0 & h^{(2)} + \mathbb{1} & 0 & 0 \\ 0 & 0 & J h^{(1)} J^* + \mathbb{1} & 0 \\ 0 & 0 & 0 & J h^{(2)} J^* + \mathbb{1} \end{pmatrix} \end{aligned}$$

is positive. Hence, for $\mathcal{B}_\varepsilon$ too we can apply Lemma 3.4 and obtain the existence of a positive constant $C_{\mathcal{B}_\varepsilon}$ such that

$$\mathbb{H}_{\mathcal{B}_\varepsilon} \;\geqslant\; -C_{\mathcal{B}_\varepsilon}.$$

By (3.38), last inequality is equivalent to

$$\mathbb{H} \;\geqslant\; \varepsilon(\mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(1)}) + \mathcal{N}_1 + \mathcal{N}_2) - C_{\mathcal{B}_\varepsilon},$$

which is the first inequality we want to prove.

To prove the second part of (3.49), we remark that, for any $\widetilde{C} > 0$,

$$\mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(2)}) + \widetilde{C}\mathcal{N}_1 + \widetilde{C}\mathcal{N}_2 - \mathbb{H} \;=\; U^*\mathbb{H}_{\widetilde{C}\mathbb{1}-\mathrm{Hess}_K}U,$$

with Hess_K defined in (3.52). Since all the $K^{(j)}$'s are bounded operators, Hess_K is bounded as well. Hence, for $\widetilde{C}$ large enough, $\widetilde{C}\mathbb{1} - \mathrm{Hess}_K > 0$. We can then apply Lemma 3.4, which ensures the existence of $C_K > 0$ such that

$$\mathbb{H}_{\widetilde{C}\mathbb{1}-\mathrm{Hess}_K} \;>\; -C_K.$$

Equivalently,

$$\mathbb{H} \;\leqslant\; \mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(2)}) + \widetilde{C}\mathcal{N}_1 + \widetilde{C}\mathcal{N}_2 + C_K. \tag{3.56}$$

Thus, (3.49) is proven by choosing $C := \max\{\varepsilon^{-1}, C_{\mathcal{B}_\varepsilon}, \widetilde{C}, C_K\}$.

From the above proof, we already recognized that $\mathbb{H} = U^*\mathbb{H}_{\mathrm{Hess}\,\mathcal{E}^{\mathrm{H}}[u_0,v_0]}U$, and all the hypotheses of Lemma 3.4 are fulfilled if $\mathcal{B} = \mathrm{Hess}\,\mathcal{E}^{\mathrm{H}}[u_0, v_0]$. Hence, a direct application of Lemma 3.4 shows that $\mathbb{H}$ can be extended to a self-adjoint operator which has a unique ground state Φ^{gs} and satisfies (3.50):

$$\inf \sigma(\mathbb{H}_{|\{\Phi^{\mathrm{gs}}\}^\perp}) \;>\; \langle \Phi^{\mathrm{gs}}, \mathbb{H}\Phi^{\mathrm{gs}}\rangle.$$

Moreover, the bounds (3.49) implies that $\mathbb{H}$ has the same form domain of the operator $\mathrm{d}\Gamma^{(1)}(h^{(1)} + 1) + \mathrm{d}\Gamma^{(2)}(h^{(2)} + 1)$. □

The estimate (3.49) will play an important role in Section 3.5 in the proof of (*iii*) and (*iv*) of Theorem 3.1.

After the identification of $\mathbb{H}$ as the second quantization of the Hessian in the sense of (3.38), the key point towards the proof of (3.49) was Lemma 3.6. This is for us a mere consequence of Assumption (A_2^{MF}) in which we require a positivity condition and the further inequality (3.3). One could relax Assumption (A_2^{MF}) by requiring the Hessian to be bounded away from zero in the first place; observe that when this is the case one should additionally require the uniqueness of the minimizer of the Hartree functional, which is for us another direct consequence of Assumption (A_2^{MF}).

A direct application of the diagonalization result of [73, Theorem 2] would allow to bound $\mathbb{H}$ from below in terms of an operator that is certainly quadratic in Z, Z^*, but not separately in a, a^* or b, b^*, thus preventing from obtaining the inequality (3.49) that is needed in the proof of Theorem 3.1. We can fix this issue by further recognizing (an observation that has no analogue for the one-component case) that the operator ξ arising in the identity (3.41) can be actually chosen to be *reduced* with respect to $\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}$, an additional feature that allows to estimate $\mathbb{H}$ from below by means of the two number operators. Such arguments are not needed for our main argument once assumption (A_2^{MF}) is taken.

3.4 Estimate in the truncated two-component Fock space

Among the claims of Theorem 3.1, the ground state energy of $\mathbb{H}$ provides the second order correction to the ground state energy of H_N^{MF}. Since $\mathbb{H}$ and H_N^{MF} act on two different spaces, respectively, $\mathcal{F}_+$ and $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, we rather compare $\mathbb{H}$ with the operator $U_N H_N^{\mathrm{MF}} U_N^*$ on $\mathcal{F}_+$, for a suitable unitary transformation U_N. This will lead to Proposition 3.8 below, the main result of this Section.

The unitary operator U_N is defined by extending ideas from [49] to the two-component setting. For arbitrary

$$\phi \in \big(\mathfrak{h}^{(1)}\big)^{\otimes_{\mathrm{sym}} j} \otimes \big(\mathfrak{h}^{(2)}\big)^{\otimes_{\mathrm{sym}} k} \qquad \text{and} \qquad \chi \in \big(\mathfrak{h}^{(1)}\big)^{\otimes_{\mathrm{sym}} \ell} \otimes \big(\mathfrak{h}^{(2)}\big)^{\otimes_{\mathrm{sym}} r}$$

we define $\phi \boxtimes \chi$ to be the function in $(h^{(1)})^{\otimes_{\mathrm{sym}}(j+\ell)} \otimes (h^{(2)})^{\otimes_{\mathrm{sym}}(k+r)}$ given by

$$\begin{aligned} (\phi \boxtimes \chi)(x_1,\dots,x_{j+\ell};y_1,\dots,y_{k+r}) \;:=\; &\frac{1}{\sqrt{j!\ell!(j+\ell!)}\sqrt{k!r!(k+r)!}} \times \\ \times \sum_{\substack{\sigma\in\Sigma_{j+\ell}\\ \pi\in\Sigma_{k+r}}} \phi(x_{\sigma_1},\dots,x_{\sigma_j};y_{\pi_1},\dots,y_{\pi_k})\, &\chi(x_{\sigma_{j+1}},\dots,x_{\sigma_{j+\ell}};y_{\pi_{k+1}},\dots,y_{\pi_{k+r}})\,, \end{aligned} \tag{3.57}$$

where Σ_p is the symmetric group of p elements. A function $\psi_N \in \mathcal{H}_{N_1,N_2,\mathrm{sym}}$ decomposes uniquely as

$$\psi_N \;=\; \sum_{j=0}^{N_1}\sum_{k=0}^{N_2} \chi_{jk} \boxtimes \big(u_0^{\otimes(N_1-j)} \otimes v_0^{\otimes(N_2-k)}\big) \tag{3.58}$$

for some $\chi_{jk} \in (\mathfrak{h}_+^{(1)})^{\otimes_{\mathrm{sym}} j} \otimes (\mathfrak{h}_+^{(2)})^{\otimes_{\mathrm{sym}} k}$, where for *each summand* of the r.h.s. of (3.58) it is understood that

$$\begin{aligned} \chi_{jk} \;&\equiv\; \chi_{jk}(x_1,\dots,x_j;y_1,\dots,y_k) \\ u_0^{\otimes(N_1-j)} \;&\equiv\; u_0(x_{j+1})\cdots u_0(x_{N_1}) \\ v_0^{\otimes(N_2-k)} \;&\equiv\; v_0(y_{k+1})\cdots v_0(y_{N_2})\,. \end{aligned}$$

Thanks to the orthogonality relations

$$\begin{aligned} \Big\langle\, \chi_{jk} \boxtimes \big(u_0^{\otimes(N_1-j)} \otimes v_0^{\otimes(N_2-k)}\big)\,,\, \chi_{\ell r} \boxtimes \big(u_0^{\otimes(N_1-\ell)} \otimes v_0^{\otimes(N_2-r)}\big) \,\Big\rangle \;&= \\ = \|\chi_{jk}\|_2^2\, \delta_{j\ell}\, \delta_{kr}\,, \end{aligned} \tag{3.59}$$

it is easy to check that

$$U_N : \mathcal{H}_{N_1,N_2,\mathrm{sym}} \longrightarrow \mathcal{F}_+^{\leqslant N}\,, \qquad U_N\psi_N \;:=\; (\chi_{jk})_{j+k\leqslant N} \tag{3.60}$$

defines a unitary operator between Hilbert spaces, where

$$\mathcal{F}_+^{\leqslant N} := \bigoplus_{L=0}^{N} \Bigg(\bigoplus_{\substack{n+m=L\\ n\leqslant N_1,\, m\leqslant N_2}} \big(\mathfrak{h}^{(1)}\big)^{\otimes_{\mathrm{sym}} n} \otimes \big(\mathfrak{h}^{(2)}\big)^{\otimes_{\mathrm{sym}} m} \Bigg). \tag{3.61}$$

The following is an analogue of the one-component result in [49, Proposition 4.2], whose proof is merely algebraic.

Proposition 3.7. *The action of the operator $U_N : \mathcal{H}_{N_1,N_2,\mathrm{sym}} \to \mathcal{F}_+^{\leqslant N}$ defined in (3.60) can be written as*

$$\big(U_N\psi_N\big)_{jk} \;=\; \Big(\big(Q^{(1)}\big)^{\otimes j} \otimes \big(Q^{(2)}\big)^{\otimes k} \frac{a_0^{N_1-j}\; b_0^{N_2-k}}{\sqrt{(N_1-j)!(N_2-k)!}}\Psi_N\Big)_{jk}, \tag{3.62}$$

where $Q^{(1)} = \mathbb{1} - |u_0\rangle\langle u_0|$, $Q^{(2)} = \mathbb{1} - |v_0\rangle\langle v_0|$, and $\Psi_N \in \mathcal{F}_+^{\leqslant N}$ is the vector whose only non-zero component coincides with ψ_N. For $\Phi \in \mathcal{F}_+^{\leqslant N}$, the adjoint of U_N acts as

$$U_N^*\,\Phi \;=\; \sum_{j=0}^{N_1}\sum_{k=0}^{N_2} \frac{1}{\sqrt{(N_1-j)!(N_2-k)!}}\Big((a_0^*)^{N_1-j}\,(b_0^*)^{N_2-k}\Phi\Big)_{N_1N_2}. \tag{3.63}$$

Moreover, for all non-zero $m,n \in \mathbb{N}$, the following identities hold true

$$\begin{aligned} U_N a_0^* a_0 U_N^* \;&=\; N_1 - \mathcal{N}_1, & U_N b_0^* b_0 U_N^* \;&=\; N_2 - \mathcal{N}_2,\\ U_N a_0^* a_m U_N^* \;&=\; \sqrt{N_1-\mathcal{N}_1}\,a_m, & U_N b_0^* b_m U_N^* \;&=\; \sqrt{N_2-\mathcal{N}_2}\,b_m,\\ U_N a_m^* a_0 U_N^* \;&=\; a_m^*\sqrt{N_1-\mathcal{N}_1}, & U_N b_m^* b_0 U_N^* \;&=\; b_m^*\sqrt{N_2-\mathcal{N}_2},\\ U_N a_m^* a_n U_N^* \;&=\; a_m^* a_n, & U_N b_m^* b_n U_N^* \;&=\; b_m^* b_n. \end{aligned} \tag{3.64}$$

Notice that, as customary, all terms in the left side of (3.64), are tacitly understood to have the form $U_N\mathfrak{I}_{N_1,N_2}^* a_0^* a_0 \mathfrak{I}_{N_1,N_2} U_N^*$ and the like, where $\mathfrak{I}_{N_1,N_2}$ is the lifting map from $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ to the Fock slice with N_1, N_2 particles.

Thanks to (3.64) we can explicitly conjugate the many-body Hamiltonian (3.10) with U_N. The main result of this Section is the following Proposition, which provides a preliminary estimate valid on the space $\mathcal{F}_+^{\leqslant M}$. The integer M satisfies the property $M \leqslant N$, and we shall suitably fix it at the end of the proof. Here and henceforth it is understood that, eventually as M and N tend to infinity, M must be chosen so as *both* $M \leqslant N_1$ and $M \leqslant N_2$.

Proposition 3.8 (Estimate on truncated Fock space)**.** *Under the same hypotheses of Theorem 3.1, given $M \leqslant N$, for any $\Phi \in \mathcal{F}_+^{\leqslant M} \cap \mathcal{D}[\mathbb{H}]$, one has*

$$\big|\langle U_N H_N^{\mathrm{MF}} U_N^* \rangle_\Phi - N e_{\mathrm{H}} - \langle \mathbb{H}\rangle_\Phi\big| \;\leqslant\; C\sqrt{\frac{M}{N}}\langle \mathbb{H} + C\rangle_\Phi \tag{3.65}$$

for a positive constant C (independent of N and M).

We refer to [49, Proposition 5.1] for the analogue in the one-component case.

Let us remark that the condition $\Phi \in \mathcal{F}_+^{\leqslant M} \cap \mathcal{D}[\mathbb{H}]$ implies, by Theorem 3.5, that Φ belongs to $\mathcal{F}_+^{\leqslant M} \cap \mathcal{D}[\mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(2)})]$. Using Assumption (A_2^{MF}), one easily sees that this implies $U_N^*\Phi \in \mathcal{D}[H_N^{\mathrm{MF}}]$, and hence (3.65) is well-defined for $\Phi \in \mathcal{F}_+^{\leqslant M} \cap \mathcal{D}[\mathbb{H}]$.

We now turn to the proof of Proposition 3.8. We first compute exactly $U_N H_N^{\mathrm{MF}} U_N^*$, which will be done in Lemma 3.9. Then, we isolate from $U_N H_N^{\mathrm{MF}} U_N^*$ the leading contribution $N e_{\mathrm{H}}$ and the second order correction $\mathbb{H}$; this will be done in Lemma 3.10. Finally, we will show that all the remaining non-relevant terms can be estimated by the right-hand side of (3.65).

Lemma 3.9. *Let us define the following five operators on the domain $\mathcal{F}^{\leqslant M} \cap \mathcal{D}[\mathbb{H}]$.*

$$\begin{aligned} M_0 \;:=&\; T_{00}^{(1)}(N_1-\mathcal{N}_1) + T_{00}^{(2)}(N_2-\mathcal{N}_2) + \frac{1}{2N}V_{0000}^{(1)}(N_1-\mathcal{N}_1)(N_1-\mathcal{N}_1-1)\\ &+ \frac{1}{2N}V_{0000}^{(2)}(N_2-\mathcal{N}_2)(N_2-\mathcal{N}_2-1) + \frac{1}{N}V_{0000}^{(12)}(N_1-\mathcal{N}_1)(N_2-\mathcal{N}_2)\\ &+ \mu_1\mathcal{N}_1 + \mu_2\mathcal{N}_2 + \frac{c_1}{2}V_{0000}^{(1)} + \frac{c_2}{2}V_{0000}^{(2)}. \end{aligned} \tag{3.66}$$

$$
\begin{aligned}
M_1 \ :=\ \sum_{m\geqslant 1}\Big[& a^*_m\sqrt{N_1-\mathcal{N}_1}\Big(T^{(1)}_{m0}+V^{(1)}_{m000}\frac{N_1-\mathcal{N}_1-1}{N}+V^{(12)}_{m000}\frac{N_2-\mathcal{N}_2}{N}\Big)\\
&+b^*_m\sqrt{N_2-\mathcal{N}_2}\Big(T^{(2)}_{m0}+V^{(2)}_{m000}\frac{N_2-\mathcal{N}_2-1}{N}+V^{(12)}_{m000}\frac{N_1-\mathcal{N}_1}{N}\Big)\\
&+\Big(T^{(1)}_{0m}+V^{(1)}_{00m0}\frac{N_1-\mathcal{N}_1-1}{N}+V^{(12)}_{00m0}\frac{N_2-\mathcal{N}_2}{N}\Big)\sqrt{N_1-\mathcal{N}_1}a_m\\
&+\Big(T^{(2)}_{0m}+V^{(2)}_{00m0}\frac{N_2-\mathcal{N}_2-1}{N}+V^{(12)}_{00m0}\frac{N_1-\mathcal{N}_1}{N}\Big)\sqrt{N_2-\mathcal{N}_2}b_m\Big].
\end{aligned}
\tag{3.67}
$$

$$
\begin{aligned}
M_2 \ :=\ \sum_{m,n\geqslant 1}\Big[& T^{(1)}_{mn}a^*_m a_n+T^{(2)}_{mn}b^*_m b_n-\mu_1\mathcal{N}_1-\mu_2\mathcal{N}_2-\frac{c_1}{2}V^{(1)}_{0000}-\frac{c_2}{2}V^{(2)}_{0000}\\
&+\frac{1}{2N}V^{(1)}_{mn00}a^*_m a^*_n\sqrt{N_1-\mathcal{N}_1}\sqrt{N_1-\mathcal{N}_1-1}\\
&+\frac{1}{2N}V^{(1)}_{00mn}\sqrt{N_1-\mathcal{N}_1-1}\sqrt{N_1-\mathcal{N}_1}a_m a_n\\
&+\frac{1}{N}V^{(1)}_{m0n0}a^*_m a_n(N_1-\mathcal{N}_1)+\frac{1}{N}V^{(1)}_{m00n}a^*_m a_n(N_1-\mathcal{N}_1)\\
&+\frac{1}{2N}V^{(2)}_{00mn}b^*_m b^*_n\sqrt{N_2-\mathcal{N}_2}\sqrt{N_2-\mathcal{N}_2-1}\\
&+\frac{1}{2N}V^{(2)}_{00mn}\sqrt{N_2-\mathcal{N}_2-1}\sqrt{N_2-\mathcal{N}_2}b_m b_n\\
&+\frac{1}{N}V^{(2)}_{m0n0}b^*_m b_n(N_2-\mathcal{N}_2)+\frac{1}{N}V^{(2)}_{m00n}b^*_m b_n(N_2-\mathcal{N}_2)\\
&+\frac{1}{N}V^{(12)}_{mn00}a^*_m b^*_n\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}\\
&+\frac{1}{N}V^{(12)}_{00mn}\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}a_m b_n\\
&+\frac{1}{N}V^{(12)}_{m0n0}a^*_m a_n(N_2-\mathcal{N}_2)+\frac{1}{N}V^{(12)}_{m00n}b^*_m b_n(N_1-\mathcal{N}_1)\\
&+\frac{1}{N}V^{(12)}_{m00n}a^*_m b_n\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}\\
&+\frac{1}{N}V^{(12)}_{m00n}\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}a_m b^*_n\Big].
\end{aligned}
\tag{3.68}
$$

$$
\begin{aligned}
M_3 \ :=\ \frac{1}{N}\sum_{m,n,q\geqslant 1}\Big[& V^{(1)}_{mnp0}a^*_m a^*_n a_p\sqrt{N_1-\mathcal{N}_1}+V^{(2)}_{mnp0}b^*_m b^*_n b_p\sqrt{N_2-\mathcal{N}_2}\\
&+V^{(12)}_{mnp0}a^*_m a_p b^*_n\sqrt{N_2-\mathcal{N}_2}+V^{(12)}_{m0np}a^*_m b^*_n b_p\sqrt{N_1-\mathcal{N}_1}\\
&+V^{(1)}_{p0mn}\sqrt{N_1-\mathcal{N}_1}a^*_p a_m a_n+V^{(2)}_{p0mn}\sqrt{N_2-\mathcal{N}_2}b^*_p b_m b_n\\
&+V^{(12)}_{p0mn}\sqrt{N_2-\mathcal{N}_2}a^*_p a_m b_n+V^{(12)}_{npm0}\sqrt{N_1-\mathcal{N}_1}a_m b^*_p b_n\Big].
\end{aligned}
\tag{3.69}
$$

$$
\begin{aligned}
M_4 \ :=\ \sum_{m,n,p,q\geqslant 1}\Big[& \frac{1}{2N}V^{(1)}_{mnpq}a^*_m a^*_n a_p a_q+\frac{1}{2N}V^{(2)}_{mnpq}b^*_m b^*_n b_p b_q\\
&+\frac{1}{N}V^{(12)}_{mnpq}a^*_m a_p b^*_n b_q\Big].
\end{aligned}
\tag{3.70}
$$

Then,

$$U_N H_N^{\mathrm{MF}} U_N^* \;=\; \sum_{j=0}^{4} M_j. \tag{3.71}$$

Proof. The proof is obtained by means of a direct computation that systematically uses the relations (3.64). Notice that the term

$$\mu_1\mathcal{N}_1 + \mu_2\mathcal{N}_2 + \frac{c_1}{2}V^{(1)}_{0000} + \frac{c_2}{2}V^{(2)}_{0000}$$

has been added in the last line of M_0 and subtracted in the first of M_2. $\square$

We now show that the relevant terms can be isolated from M_0 and M_2 and that there is an exact cancellation in M_1, due to the fact that (u_0, v_0) is the minimizer of the Hartree functional.

Lemma 3.10. *For M_0, M_1, M_2 defined in* (3.66)-(3.70), *one has the following re-arrangements.*

(i) (Isolation of the leading term from M_0)

$$\begin{aligned} M_0 \;&= N e_{\mathrm{H}} + \frac{1}{2N}V^{(1)}_{0000}\,\mathcal{N}_1(\mathcal{N}_1+1) + \frac{1}{2N}V^{(2)}_{0000}\,\mathcal{N}_2(\mathcal{N}_2+1) \\ &\quad + \frac{1}{N}V^{(12)}_{0000}\,\mathcal{N}_1\mathcal{N}_2. \end{aligned} \tag{3.72}$$

(ii) (Cancellation of the linear contribution to M_1)

$$\begin{aligned} M_1 \;=\; \frac{1}{N}\sum_{m\geqslant 1}\Big[&- V^{(1)}_{m000}a_m^*\sqrt{N_1-\mathcal{N}_1}\,(\mathcal{N}_1+1) - V^{(2)}_{m000}b_m^*\sqrt{N_2-\mathcal{N}_2}\,(\mathcal{N}_2+1) \\ &- V^{12}_{m000}a_m^*\sqrt{N_1-\mathcal{N}_1}\,\mathcal{N}_2 - V^{(12)}_{0m00}b_m^*\sqrt{N_2-\mathcal{N}_2}\mathcal{N}_1 \\ &- V^{(1)}_{00m0}(\mathcal{N}_1+1)\sqrt{N_1-\mathcal{N}_1}a_m - V^{(2)}_{00m0}\,(\mathcal{N}_2+1)\sqrt{N_2-\mathcal{N}_2}b_m \\ &- V^{12}_{00m0}\,\sqrt{N_1-\mathcal{N}_1}\,\mathcal{N}_2\,a_m - V^{(12)}_{000m}\,\mathcal{N}_1\sqrt{N_2-\mathcal{N}_2}\,b_m\Big]. \end{aligned} \tag{3.73}$$

(iii) (Isolation of the Bogoliubov Hamiltonian from M_2)

$$
\begin{aligned}
M_2 \;=\; \mathbb{H} + \sum_{m,n\geqslant 1} \Big(& \frac{1}{2} V^{(1)}_{mn00} a^*_m a^*_n \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_1-\mathcal{N}_1-1}-N_1}{N} \\
& \frac{1}{2} V^{(1)}_{00mn} \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_1-\mathcal{N}_1-1}-N_1}{N} a_m a_n \\
& + \frac{1}{N}\big(V^{(1)}_{mn0} + V^{(1)}_{m00n}\big) a^*_m a_n (1-\mathcal{N}_1) \\
& + \frac{1}{2} V^{(2)}_{mn00} b^*_m b^*_n \frac{\sqrt{N_2-\mathcal{N}_2}\sqrt{N_2-\mathcal{N}_2-1}-N_2}{N} \\
& + \frac{1}{2} V^{(2)}_{00mn} \frac{\sqrt{N_2-\mathcal{N}_2}\sqrt{N_2-\mathcal{N}_2-1}-N_2}{N} b_m b_n \\
& + \frac{1}{N}\big(V^{(2)}_{m0n0} + V^{(2)}_{m00n}\big) b^*_m b_n (1-\mathcal{N}_2) \\
& + V^{(12)}_{mn00} a^*_m b^*_n \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}-\sqrt{N_1 N_2}}{N} \\
& + V^{(12)}_{00mn} \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}-\sqrt{N_1 N_2}}{N} a_m b_n \\
& - \frac{1}{N} V^{(12)}_{m0n0} a^*_m a_n \mathcal{N}_2 - \frac{1}{N} V^{(12)}_{0m0n} b^*_m b_n \mathcal{N}_1 \\
& + V^{(12)}_{m00n} a^*_m b_n \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}-\sqrt{N_1 N_2}}{N} \\
& + V^{(12)}_{0nm0} \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2}-\sqrt{N_1 N_2}}{N} a_m b^*_n \Big).
\end{aligned}
\tag{3.74}
$$

Proof. We recall that the minimum of the Hartree functional is

$$
e_{\mathrm{H}} \;=\; c_1 T^{(1)}_{00} + c_2 T^{(2)}_{00} + \frac{c_1^2}{2} V^{(1)}_{0000} + \frac{c_2^2}{2} V^{(2)}_{0000} + c_1 c_2 V^{(12)}_{0000}. \tag{3.75}
$$

A direct computation then yields (3.72).

To prove (3.73), we note that, since (u_0, v_0) minimizes the Hartree functional, we have the identities

$$
\begin{aligned}
T^{(1)}_{m0} + c_1 V^{(1)}_{m000} + c_2 V^{(12)}_{m000} \;&=\; 0 \\
T^{(2)}_{m0} + V^{(2)}_{m000} + c_1 V^{(12)}_{m000} \;&=\; 0.
\end{aligned}
\tag{3.76}
$$

Since $c_i = N_i/N$, last two identities yield an exact cancellation in M_1: for example, the contribution coming from the first line of the r.h.s. of (3.67) reduces to

$$
\frac{1}{N}\sum_{m\geqslant 1}\Big[- V^{(1)}_{m000} a^*_m \sqrt{N_1-\mathcal{N}_1}\,(\mathcal{N}_1+1) - V^{(2)}_{m000} b^*_m \sqrt{N_2-\mathcal{N}_2}\,(\mathcal{N}_2+1)\Big].
$$

This allows us to bring M_1 to the form (3.73).

Finally, (3.74) is obtained by a mere regrouping of terms. For example, the contribution from the second line of (3.68) can be rewritten as

$$
\frac{c_1}{2}\sum_{m,n\geqslant 1} V^{(1)}_{mn00} a^*_m a^*_n + \frac{1}{2}\sum_{m,n\geqslant 1} V^{(1)}_{mn00} a^*_m a^*_n \frac{\sqrt{N_1-\mathcal{N}_1}\sqrt{N_1-\mathcal{N}_1-1}-N_1}{N},
$$

having isolated the N-independent contribution. The same is done for all the other summands of (3.68). Recalling the definition (3.15) of $\mathbb{H}$, the outcome is (3.74). □

The final step in order to prove Proposition 3.8 is the following Lemma, that provides the appropriate estimate for all the remainders $M_0 - Ne_{\mathrm{H}}$, M_1, $M_2 - \mathbb{H}$, M_3, and M_4.

Lemma 3.11. *There exists a constant $C > 0$ such that, for any $\Phi \in \mathcal{F}_+^{\leqslant M} \cap \mathcal{D}[\mathbb{H}]$*

$$\big|\langle M_0\rangle_\Phi - Ne_{\mathrm{H}}\big| \;\leqslant\; C\frac{M}{N}\langle\mathcal{N}\rangle_\Phi \tag{3.77}$$

$$|\langle M_1\rangle_\Phi| \;\leqslant\; C\sqrt{\frac{M}{N}}\langle\mathcal{N}\rangle_\Phi \tag{3.78}$$

$$\big|\langle M_2\rangle_\Phi - \langle\mathbb{H}\rangle_\Phi\big| \;\leqslant\; C\frac{M}{N}\langle\mathcal{N}\rangle_\Phi \tag{3.79}$$

$$|\langle M_3\rangle_\Phi| \;\leqslant\; C\sqrt{\frac{M}{N}}\Big(\langle\mathbb{H}\rangle_\Phi + \langle\mathcal{N}\rangle_\Phi + C\Big) \tag{3.80}$$

$$|\langle M_4\rangle_\Phi| \;\leqslant\; C\frac{M}{N}\Big(\langle\mathbb{H}\rangle_\Phi + \langle\mathcal{N}\rangle_\Phi + C\Big) \tag{3.81}$$

Let us postpone the proof of Lemma 3.11 and now conclude.

Proof of Theorem 3.8. Let us fix $\Phi \in \mathcal{F}_+^{\leqslant M} \cap \mathcal{D}[\mathbb{H}]$. By Lemma 3.9 we get

$$\langle U_N H_N U_N^*\rangle_\Phi \;=\; Ne_{\mathrm{H}} + \langle\mathbb{H}\rangle_\Phi + \langle M_0 - Ne_{\mathrm{H}}\rangle_\Phi + \langle M_1\rangle_\Phi + \langle M_2 - \mathbb{H}\rangle_\Phi + \langle M_3\rangle_\Phi + \langle M_4\rangle_\Phi,$$

and hence, applying Lemma 3.11, we find

$$\big|\langle U_N H_N^{\mathrm{MF}} U_N^*\rangle_\Phi - Ne_{\mathrm{H}} - \langle\mathbb{H}\rangle_\Phi\big| \;\leqslant\; C\sqrt{\frac{M}{N}}\big(2\langle\mathbb{H}\rangle_\Phi + 5\langle\mathcal{N}\rangle_\Phi + 2C\big), \tag{3.82}$$

having used $M/N \leqslant \sqrt{M/N}$. Using positivity of $h^{(1)}$ and $h^{(2)}$ and Theorem 3.5, one finds

$$\mathcal{N} \leqslant \mathcal{N} + \mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(2)}) \;\leqslant\; C\,\mathbb{H} + C^2.$$

This yields the bound

$$\big|\langle U_N H_N^{\mathrm{MF}} U_N^*\rangle_\Phi - Ne_{\mathrm{H}} - \langle\mathbb{H}\rangle_\Phi\big| \;\leqslant\; C\sqrt{\frac{M}{N}}\big(\langle\mathbb{H}\rangle_\Phi + C\big), \tag{3.83}$$

for a suitable constant C. □

Only Lemma 3.11 remains to be proven. We first state a technical Lemma that we will use through the proof.

Lemma 3.12. *Under the same assumptions of Theorem 3.1,*

$$\mathrm{d}\Gamma^{(i)}(T^{(j)}) \;\leqslant\; \alpha\mathbb{H} + \alpha\mathcal{N} + \alpha, \qquad \textit{for } j \in \{1,2\} \tag{3.84}$$

$$\mathrm{d}\Gamma^{(1)}\Big(|V^{(12)}| * |v_0|^2\Big) \;\leqslant\; \beta\mathcal{N} \tag{3.85}$$

$$\mathrm{d}\Gamma^{(2)}\Big(|V^{(12)}| * |u_0|^2\Big) \;\leqslant\; \gamma\mathcal{N} \tag{3.86}$$

for positive constants α, β, γ.

Proof. Let us prove (3.84) for the case $j=1$. By assumption (A_2^{MF}) we know that, for every $\varepsilon>0$, $V^{(1)} \geqslant -\varepsilon\, C^{(1)}(1-\Delta)-\varepsilon^{-1}$ and $V^{(12)} \geqslant -\varepsilon\, C^{(12)}(1-\Delta)-\varepsilon^{-1}$. Hence, we deduce

$$V^{(1)} * |u_0|^2 \;\geqslant\; -\varepsilon C^{(1)} - \varepsilon C^{(1)}(-\Delta) - \varepsilon C^{(1)} \|u_0\|^2_{H^1} - \varepsilon^{-1} \tag{3.87}$$

and

$$V^{(12)} * |v_0|^2 \;\geqslant\; -\varepsilon C^{(12)} - \varepsilon C^{(12)}(-\Delta) - \varepsilon C^{(12)} \|v_0\|^2_{H^1} - \varepsilon^{-1}. \tag{3.88}$$

By recalling the definition of $h^{(1)}$ from (3.13), the last two estimates imply the existence of a constant $\widetilde{\alpha}>0$ large enough such that

$$T^{(1)} \;\leqslant\; \widetilde{\alpha} h^{(1)} + \widetilde{\alpha}. \tag{3.89}$$

Taking the second quantization $\mathrm{d}\Gamma^{(1)}(\cdot)$ of both sides and using (3.49) we obtain (3.84) for $\alpha>0$ big enough. The same holds for $T^{(2)}$.

To prove (3.85) it is enough to note that, by Assumption (A_2^{MF}), the multiplication operator $V^{(12)} * |v_0|^2$ is bounded. The desired inequality is hence trivial, since the second quantization of a bounded positive operator is always estimated by a multiple of the number operator. An analogous proof holds for (3.86).

□

Proof of Lemma 3.11. Let us write

$$\langle M_0 - N e_{\mathrm{H}} \rangle_\Phi \;=\; M_0^{(1)} + M_0^{(2)} + M_0^{(12)} \tag{3.90}$$

$$\langle M_1 \rangle_\Phi \;=\; M_1^{(1)} + M_1^{(2)} + M_1^{(12)} \tag{3.91}$$

$$\langle M_2 - \mathbb{H} \rangle_\Phi \;=\; M_2^{(1)} + M_2^{(2)} + M_2^{(12)} \tag{3.92}$$

$$\langle M_3 \rangle_\Phi \;=\; M_3^{(1)} + M_3^{(2)} + M_3^{(12)} \tag{3.93}$$

$$\langle M_4 \rangle_\Phi \;=\; M_4^{(1)} + M_4^{(2)} + M_4^{(12)}, \tag{3.94}$$

where, in self-explanatory notation, each summand with label (α) contains all the terms depending on the interaction potential $V^{(\alpha)}$. We will estimate the $M_k^{(12)}$'s; all the other terms do not involve interactions between particles of different type, and hence, they are on the same footing as the terms estimated in [49, Proposition 5.2].

Let us consider $M_0^{(12)}$. Since $\Phi \in \mathcal{F}_+^{\leqslant M}$, we have $\langle \mathcal{N}_i \rangle_\Phi \leqslant \langle \mathcal{N} \rangle_\Phi \leqslant M$, and hence

$$\big|M_0^{(12)}\big| \;=\; \Big|V^{(12)}_{0000} \langle \frac{\mathcal{N}_1 \mathcal{N}_2}{N} \rangle_\Phi \Big| \;\leqslant\; \mathcal{K}_0 \frac{M}{N} \langle \mathcal{N} \rangle_\Phi, \tag{3.95}$$

for $\mathcal{K}_0 = |V^{(12)}_{0000}|$.

Let us now consider $M_1^{(12)}$. By a Cauchy-Schwarz inequality we write

$$\begin{aligned}
\Big| \sum_{m\geqslant 1} V^{(12)}_{m000} \frac{1}{N} \langle a_m^* \sqrt{N_1 - \mathcal{N}_1} \mathcal{N}_2 \rangle_\Phi + \mathrm{h.\,c.} \Big| \;&\leq\; \frac{2}{N} \Big(\sum_{m\geqslant 1} |V^{(12)}_{m000}|^2 \Big)^{1/2} \\
&\qquad \times \Big(\sum_{m\geqslant 1} \langle a_m^* a_m \rangle_\Phi \langle (N_1 - \mathcal{N}_1) \mathcal{N}_2^2 \rangle_\Phi \Big)^{1/2} \\
&\leqslant\; \frac{2\, \|K^{(12)}\|_{\mathrm{HS}}}{N} \Big(N \langle \mathcal{N} \rangle_\Phi \langle \mathcal{N}^2 \rangle_\Phi \Big)^{1/2} \\
&\leqslant\; 2\, \|K^{(12)}\|_{\mathrm{HS}} \sqrt{\frac{M}{N}} \langle \mathcal{N} \rangle_\Phi.
\end{aligned}$$

In the second and third step we have used $N_1 \leqslant N$, positivity of $\mathcal{N}_1$, the inequality $\langle \mathcal{N} \rangle_\Phi \leqslant M$, together with the property

$$\begin{aligned}\sum_{m\geqslant 1} |V^{(12)}_{m000}|^2 \;&=\; \sum_{m\geqslant 1} |\langle u_m, K^{(12)} u_0\rangle|^2 \;=\; \sum_{m\geqslant 1} \langle u_m, K^{(12)} u_0\rangle\, \langle u_0, K^{(12)} u_m\rangle \\ &\leqslant\; \|K^{(12)}\|^2_{\mathrm{HS}} < +\infty.\end{aligned}$$

There is another summand in $M_1^{(12)}$, but it differs from the one we just estimated only by the interchange of the two components; for this reason, we omit the details of its estimate. Thus,

$$|M_1^{(12)}| \;\leqslant\; 4\|K^{(12)}\|^2_{\mathrm{HS}} \sqrt{\frac{M}{N}}\langle \mathcal{N}\rangle_\Phi. \tag{3.96}$$

Let us consider $M_2^{(12)}$, whose expression is

$$\begin{aligned} M_2^{(12)} \;=\; &\sum_{m,n\geqslant 1} \Big[\frac{1}{N} V^{(12)}_{mn00} \langle a_m^* b_n^* \big(\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2} - \sqrt{N_1 N_2}\big)\rangle_\Phi + \mathrm{h.\,c.}\Big] &(3.97)\\ &- \sum_{m,n\geqslant 1}\Big[\frac{1}{N} V^{(12)}_{m0n0}\langle a_m^* a_n \mathcal{N}_2\rangle_\Phi\Big] &(3.98)\\ &- \sum_{m,n\geqslant 1}\Big[\frac{1}{N} V^{(12)}_{0m0n}\langle b_m^* b_n \mathcal{N}_1\rangle_\Phi\Big] &(3.99)\\ &+ \sum_{m,n\geqslant 1}\Big[\frac{1}{N} V^{(12)}_{m00n}\langle a_m^* b_n \big(\sqrt{N_1-\mathcal{N}_1}\sqrt{N_2-\mathcal{N}_2} - \sqrt{N_1 N_2}\big)\rangle_\Phi + \mathrm{h.\,c.}\Big], &(3.100)\end{aligned}$$

and let us treat the four summands one by one. First let us define the operator

$$X \;:=\; \sqrt{\frac{N_1-\mathcal{N}_1}{N_1}}\sqrt{\frac{N_2-\mathcal{N}_2}{N_2}}.$$

By a Cauchy-Schwarz inequality we get

$$\begin{aligned}|(3.97)| \;&\leqslant\; 2\sqrt{\frac{N_1N_2}{N^2}}\Big(\sum_{m,n\geqslant 1}|\langle u_m, K^{(12)}\overline{v_n}\rangle|^2\Big)^{1/2}\Big(\sum_{m,n\geqslant 1}\langle a_m^* b_n^* a_m b_n\rangle_\Phi\Big)^{1/2}\big\langle\,(X-\mathbb{1})^2\,\big\rangle_\Phi^{1/2}\\ &\leqslant 2\sqrt{\frac{N_1N_2}{N^2}}\Big(\sum_{m\geqslant 1}\langle u_m, \big|K^{(12)}\big|^2 u_m\rangle\Big)^{1/2}\langle \mathcal{N}_1\mathcal{N}_2\rangle_\Phi^{1/2}\Big\langle\Big(-\frac{\mathcal{N}_1}{N_1}-\frac{\mathcal{N}_2}{N_2}+\frac{\mathcal{N}_1\mathcal{N}_2}{N_1N_2}\Big)^2\Big\rangle_\Phi^{1/2},\end{aligned}$$

having used the estimate $(X-\mathbb{1})^2 \leqslant (X^2-\mathbb{1})^2$. Now, using $N_1N_2 \leqslant N^2$, $\langle \mathcal{N}_i\rangle_\Phi \leqslant \langle \mathcal{N}\rangle_\Phi \leqslant M$, and the fact that $K^{(12)}$ is Hilbert-Schmidt, we obtain

$$|(3.97)| \;\leqslant 2\|K^{(12)}\|_{\mathrm{HS}}\,\frac{M^{1/2}}{N_1N_2}\langle \mathcal{N}\rangle_\Phi^{1/2}\big\langle\big(N_2\mathcal{N}_1 + N_1\mathcal{N}_2 - \mathcal{N}_1\mathcal{N}_2\big)^2\big\rangle^{1/2}.$$

Since $\mathcal{N}_1\mathcal{N}_2 \leqslant N_2\mathcal{N}_1 + N_1\mathcal{N}_2$ on $\mathcal{F}_+^{\leqslant M}$, we finally get

$$|(3.97)| \;\leqslant 4\|K^{(12)}\|_{\mathrm{HS}}\,\frac{M^{1/2}}{N_1N_2}\langle \mathcal{N}\rangle_\Phi^{1/2}\big\langle\big(N_2\mathcal{N}_1 + N_1\mathcal{N}_2\big)^2\big\rangle^{1/2} \;\leqslant\; \widetilde{\mathcal{K}_2}\,\frac{M}{N}\langle \mathcal{N}\rangle_\Phi, \tag{3.101}$$

for some $\widetilde{\mathcal{K}_2} > 0$.

To estimate (3.98) we note that

$$(3.98) \;=\; -\Big\langle \mathrm{d}\Gamma^{(1)}(V^{(12)} * |v_0|^2)\frac{\mathcal{N}_2}{N}\Big\rangle_\Phi,$$

and, by (3.85),

$$|(3.98)| \;\leqslant\; \beta\frac{M}{N}\langle\mathcal{N}\rangle_\Phi. \tag{3.102}$$

Analogously,

$$|(3.99)| \;\leqslant\; \gamma\frac{M}{N}\langle\mathcal{N}\rangle_\Phi \tag{3.103}$$

for γ given by (3.86).

To estimate (3.100) we write

$$(3.100) \;=\; \frac{1}{N}\sum_{\substack{j\geqslant 1,\ k\geqslant 0\\ j+k\leqslant M}} j(k+1)\langle\Phi_{j,k}, K^{(12)}_{1,1}\Phi_{j-1,k+1}\rangle + \mathrm{h.\,c.},$$

where $\Phi = (\Phi_{j,k})_{jk} \in \mathcal{F}_+^{\leqslant M}$ and $K^{(12)}_{1,1}$ is the integral operator $K^{(12)}$ defined in (3.46) and taken with kernel $K^{(12)}(x_1, y_1)$. By using Cauchy-Schwarz we get

$$\begin{aligned}|(3.100)| \;&\leqslant \frac{2}{N}\sum_{\substack{j\geqslant 1,\ k\geqslant 0\\ j+k\leqslant M}} j(k+1)\Big(\langle\Phi_{j,k},\Phi_{j,k}\rangle + \|K^{(12)}\|^2_{\mathrm{op}}\langle\Phi_{j-1,k+1},\Phi_{j-1,k+1}\rangle\Big)\\ &= \frac{2}{N}(1+\|K^{(12)}\|_{\mathrm{op}})\langle\Phi, \mathcal{N}_1(\mathcal{N}_2+1)\Phi\rangle,\end{aligned}$$

and hence, the inequality $\mathcal{N}_i \leqslant \mathcal{N} \leqslant M$ valid on $\mathcal{F}_+^{\leqslant M}$ yields

$$|(3.100)| \;\leqslant\; \mathcal{K}_2'\frac{M}{N}\langle\mathcal{N}\rangle_\Phi, \tag{3.104}$$

for some $\mathcal{K}_2' > 0$. Putting together (3.101), (3.102), (3.103), and (3.104) we conclude

$$\big|M_2^{(12)}\big| \;\leqslant\; \mathcal{K}_2\frac{M}{N}\langle\mathcal{N}\rangle_\Phi, \tag{3.105}$$

with $\mathcal{K}_2 := \widetilde{\mathcal{K}_2} + \beta + \gamma + \mathcal{K}_2'$.

Let us consider $M_3^{(12)}$, whose expression is

$$M_3^{(12)} \;=\; \sum_{m,n,p\geqslant 1}\Big[\frac{1}{N}V^{(12)}_{mnp0}\langle a^*_m a_p b^*_n\sqrt{N_2-\mathcal{N}_2}\rangle_\Phi + \mathrm{h.\,c.}\Big] \tag{3.106}$$

$$+ \sum_{m,n,p\geqslant 1}\Big[\frac{1}{N}V^{(12)}_{m0np}\langle a^*_m b^*_n b_p\sqrt{N_1-\mathcal{N}_1}\rangle_\Phi + \mathrm{h.\,c.}\Big]. \tag{3.107}$$

First, we notice that

$$(3.106) \;=\; \langle\Phi, U_N\sum_{j=1}^{N_1}\sum_{k=1}^{N_2} Q^{(1)}_{x_j}\otimes Q^{(2)}_{y_k}V^{(12)}(x_j-y_k)Q^{(1)}_{x_j}\otimes P^{(2)}_{y_k}U_N^*\,\Phi\rangle + \mathrm{h.\,c.}\,. \tag{3.108}$$

Now, by splitting $V^{(12)}$ into positive and negative part and using Cauchy-Schwarz, one obtains the inequality

$$\begin{aligned}Q_x^{(1)} \otimes Q_y^{(2)} V^{(12)}(x-y) Q_x^{(1)} \otimes P_y^{(2)} + Q_x^{(1)} \otimes P_y^{(2)} V^{(12)}(x-y) Q_x^{(1)} \otimes Q_y^{(2)} \\ \leqslant \varepsilon^{-1} Q_x^{(1)} \otimes Q_y^{(2)} \big|V^{(12)}(x-y)\big| Q_x^{(1)} \otimes Q_y^{(2)} \\ + \varepsilon\, Q_x^{(1)} \otimes P_y^{(2)} \big|V^{(12)}(x-y)\big| Q_x^{(1)} \otimes P_y^{(2)},\end{aligned} \tag{3.109}$$

whence, substituting into (3.108), one gets

$$\begin{aligned}(3.106) \;\leqslant\; & \frac{1}{\varepsilon N} \sum_{m,n,p,q \geqslant 1} \big|V^{(12)}\big|_{mnpq} \langle a_m^* b_n^* a_p b_q \rangle_\Phi \\ & + \frac{\varepsilon}{N} \big\langle \mathrm{d}\Gamma^{(1)}\Big(\big|V^{(12)}\big| * |v_0|^2\Big)(N_2 - \mathcal{N}_2)\big\rangle_\Phi\end{aligned} \tag{3.110}$$

for some $\varepsilon > 0$ that we are going to specify in a moment. We first focus on the first summand of the r.h.s of (3.110). Using the expression in components $\Phi = (\Phi_{j,k})_{jk} \in \mathcal{F}_+^{\leqslant M}$, we can write

$$\begin{aligned}\frac{1}{\varepsilon N} \sum_{m,n,p,q \geqslant 1} \big|V^{(12)}_{mnpq}\big| \langle \Phi, a_m^* a_p b_n^* b_q \Phi \rangle \;&=\; \frac{1}{\varepsilon N} \sum_{\substack{j,k \geqslant 1, \\ j+k \leqslant M}} jk \langle \Phi_{j,k}, \big|V(x_1 - y_1)\big| \Phi_{j,k} \rangle \\ &\leqslant\; \frac{C^{(12)}}{\varepsilon N} \sum_{\substack{j,k \geqslant 1, \\ j+k \leqslant M}} jk \langle \Phi_{j,k}, \big(1 - \Delta_{x_1} - \Delta_{y_1}\big) \Phi_{j,k} \rangle \\ &=\; \frac{C^{(12)}}{\varepsilon N} \langle \Phi, \big(\mathcal{N}_1 \mathcal{N}_2 + \mathrm{d}\Gamma^{(1)}(T^{(1)}) \mathcal{N}_2 + \mathcal{N}_1 \mathrm{d}\Gamma^{(2)}(T^{(2)})\big) \Phi \rangle,\end{aligned}$$

having used Assumption (A_2^{MF}) in the second step. Thanks to the inequality $\mathcal{N}_i \leqslant \mathcal{N} \leqslant M$ valid on $\mathcal{F}_+^{\leqslant M}$ and Lemma 3.12, we obtain

$$\frac{1}{\varepsilon N} \sum_{mnpq} |V^{(12)}_{mnpq}| \langle \Phi, a_m^* b_n^* a_p b_q \Phi \rangle \;\leqslant\; \widetilde{\mathcal{K}_3} \frac{M}{\varepsilon N} \big(\langle \mathcal{N} \rangle_\Phi + \langle \mathbb{H} \rangle_\Phi + \widetilde{\mathcal{K}_3}\big),$$

for some $\widetilde{\mathcal{K}_3} > 0$. The second summand in the r.h.s of (3.110), in turn, is estimated using (3.85) as

$$\frac{\varepsilon}{N} \big\langle \Phi, \mathrm{d}\Gamma^{(1)}\Big(\big|V^{(12)}\big| * |v_0|^2\Big)(N_2 - \mathcal{N}_2)\big\rangle_\Phi \;\leqslant\; \alpha\varepsilon\big(\langle \mathcal{N} \rangle_\Phi + \langle \mathbb{H} \rangle_\Phi\big).$$

By finally choosing $\varepsilon = (M/N)^{1/2}$, the last two inequalities yield

$$|(3.106)| \;\leqslant\; (\widetilde{\mathcal{K}_3} + \alpha) \sqrt{\frac{M}{N}} \big(\langle \mathcal{N} \rangle_\Phi + \langle \mathbb{H} \rangle_\Phi + \widetilde{\mathcal{K}_3}\big).$$

The term (3.107) differs from (3.106) only by the exchange of the two components, and hence, it is treated analogously. This yields

$$\big|M_3^{(12)}\big| \;\leqslant\; \mathcal{K}_3 \sqrt{\frac{M}{N}} \big(\langle \mathcal{N} \rangle_\Phi + \langle \mathbb{H} \rangle_\Phi + \mathcal{K}_3\big), \tag{3.111}$$

for a positive constant $\mathcal{K}_3$ big enough.

Let us finally consider $M_4^{(12)}$. Using $\Phi = (\Phi_{j,k})_{jk}$, we can write

$$\begin{aligned} M_4^{(12)} &= \frac{1}{N} \sum_{\substack{j,k\geqslant 1\\ j+k\leqslant M}} jk\langle \Phi_{j,k}, V(x_1-y_1)\Phi_{j,k}\rangle \\ &\leqslant \frac{C^{(12)}}{N} \sum_{\substack{j,k\geqslant 1\\ j+k\leqslant M}} jk\langle \Phi_{j,k}, \big(1-\Delta_{x_1}-\Delta_{y_1}\big)\Phi_{j,k}\rangle \\ &\leqslant \frac{C^{(12)}}{N}\langle \Phi, \big(\mathcal{N}_1\mathcal{N}_2 + \mathrm{d}\Gamma^{(1)}(T^{(1)})\mathcal{N}_2 + \mathcal{N}_1\mathrm{d}\Gamma^{(2)}(T^{(2)})\big)\Phi\rangle, \end{aligned}$$

having used Assumption (A_2^{MF}) in the second step. By the inequality $\mathcal{N}_i \leqslant \mathcal{N} \leqslant M$, valid on $\mathcal{F}_+^{\leqslant M}$ and (3.84), we get

$$M_4^{(12)} \;\leqslant\; \mathcal{K}_4 \frac{M}{N}\big(\langle \mathcal{N}\rangle_\Phi + \langle \mathbb{H}\rangle_\Phi + \mathcal{K}_4\big), \tag{3.112}$$

for some constant $\mathcal{K}_4 > 0$.

Eqs. (3.95), (3.96), (3.105), (3.111), and (3.112), together with their analogous for the terms depending on $V^{(1)}$ and $V^{(2)}$ yield the desired claim, provided that the overall constant C is chosen large enough. □

3.5 Proof of energy convergence and ground state norm approximation

We are now ready to complete the proof of Theorem 3.1 by proving the statements (iii) and (iv).

3.5.1 Localization in Fock space

Proposition 3.8 provides an estimate for the expectation value of the difference $U_N H_N^{\mathrm{MF}} U_N^* - Ne_{\mathrm{H}} - \mathbb{H}$ in the truncated space $\mathcal{F}_+^{\leqslant M}$. In what follows we recall a result that allows us to localize the energy of a state in the space $\mathcal{F}_+^{\leqslant M}$. As we shall see, at the end of the proof we will be able to choose $M \ll N$ in such a way that the localization produces only negligible remainders. This idea goes back to [50, Theorem A.1] and we will follow the simplified presentation in [49, Proposition 6.1].

Consider two smooth, real functions f and g such that $0 \leqslant f, g \leqslant 1$, $f^2 + g^2 = 1$, $f(x) = 1$ for $|x| \leq 1/2$, and $f(x) = 0$ for $|x| \geqslant 1$. By spectral calculus, we define

$$\begin{aligned} f_M &:= f(\mathcal{N}/M) \\ g_M &:= g(\mathcal{N}/M). \end{aligned} \tag{3.113}$$

Let us also define the orthogonal projection $\mathcal{P}_L$ onto the sector of $\mathcal{F}_+$ with exactly L particles, namely the subspace

$$\bigoplus_{\substack{j\geqslant 0,\, k\geqslant 0\\ j+k=L}} \big(\mathfrak{h}_+^{(1)}\big)^{\otimes_{\mathrm{sym}} j} \otimes \big(\mathfrak{h}_+^{(2)}\big)^{\otimes_{\mathrm{sym}} k} \;=\; U^*\Big(\big(\mathfrak{h}_+^{(1)} \oplus \mathfrak{h}_+^{(2)}\big)^{\otimes_{\mathrm{sym}} L}\Big).$$

Here $U : \mathcal{F}_+ \to \mathcal{G}_+$ is the unitary operator given by Theorem 3.3.

Proposition 3.13. *Let A be a non-negative operator on $\mathcal{F}_+$ such that $\mathcal{P}_L\mathcal{D}(A) \subset \mathcal{D}(A)$ for any $L \in \mathbb{N}$. Suppose moreover that there exists $\sigma \geqslant 0$ such that $\mathcal{P}_L A \mathcal{P}_{L'} = 0$ when $|L - L'| > \sigma$. Then*

$$\pm\, A - f_M A f_M - g_M A g_M \;\leqslant\; \frac{C_f \sigma^3}{M^2} A_0, \tag{3.114}$$

where $A_0 := \sum_{L\in\mathbb{N}} \mathcal{P}_L A \mathcal{P}_L$ and C_f is a positive constant depending only on f.

This result is a variant of the IMS formula, that can be found in [49, Proposition 6.1], which is, in turn, an adaptation of [50, Theorem A.1]. As a direct consequence of Proposition 3.13, the next Lemma provides the precise estimates that enable to localize the energy of a state in $\mathcal{F}_+^{\leqslant N}$ into the subspace $\mathcal{F}_+^{\leqslant M}$.

Let us define the operator

$$\widetilde{H}_N^{\mathrm{MF}} \;:=\; U_N H_N^{\mathrm{MF}} U_N^* - N e_{\mathrm{H}}. \tag{3.115}$$

Let ψ_N^{gs} be the ground state of H_N^{MF}, whose existence and uniqueness (up to a phase) are discussed after Theorem 3.1. Then, by unitarity,

$$\Phi_N \;:=\; U_N \psi_N^{\mathrm{gs}} \tag{3.116}$$

is the unique (up to a phase) ground state of $\widetilde{H}_N^{\mathrm{MF}}$. We will use the following notations for the ground state energies of $\widetilde{H}_N^{\mathrm{MF}}$ and $\mathbb{H}$

$$\begin{aligned} \lambda(\widetilde{H}_N^{\mathrm{MF}}) \;&:= \langle \Phi_N, \widetilde{H}_N^{\mathrm{MF}} \Phi_N\rangle = E_N^{\mathrm{MF}} - N e_{\mathrm{H}} \\ \lambda(\mathbb{H}) \;&:= \langle \Phi^{\mathrm{gs}}, \mathbb{H}\Phi^{\mathrm{gs}}\rangle. \end{aligned} \tag{3.117}$$

Lemma 3.14. *There exist positive constants κ_1, κ_2 such that, for any $M \leqslant N$,*

$$\pm\big(\mathbb{H} - f_M \mathbb{H} f_M - g_M \mathbb{H} g_M\big) \;\leqslant\; \frac{\kappa_1}{M^2}(\mathbb{H} + \kappa_1) \tag{3.118}$$

and

$$\pm\big(\widetilde{H}_N^{\mathrm{MF}} - f_M \widetilde{H}_N^{\mathrm{MF}} f_M - g_M \widetilde{H}_N^{\mathrm{MF}} g_M\big) \;\leqslant\; \frac{\kappa_2}{M^2}\big(\widetilde{H}_N^{\mathrm{MF}} + \kappa_2 N\big). \tag{3.119}$$

Proof. To prove (3.118), we apply Proposition 3.13 with $A = \mathbb{H} - \lambda(\mathbb{H}) \geqslant 0$ and $\sigma = 2$. All is needed is the computation of the corresponding A_0. We notice that

$$\sum_{L=0}^{\infty} \mathcal{P}_L\big(\mathbb{H} - \lambda(\mathbb{H})\big)\mathcal{P}_L \;=\; U^* \mathrm{d}\Gamma(\mathcal{B}_1) U - \lambda(\mathbb{H}),$$

where

$$\mathcal{B}_1 \;=\; \begin{pmatrix} h^{(1)} + c_1 K^{(1)} & \sqrt{c_1 c_2} K^{(12)} \\ \sqrt{c_1 c_2} K^{(12)*} & h^{(2)} + c_2 K^{(2)} \end{pmatrix},$$

$\mathrm{d}\Gamma(\cdot)$ is defined in (3.31), and U is given by Theorem 3.3. Since the $K^{(j)}$'s are bounded, there exists $\widetilde{\kappa_1} > 0$ (depending on $\lambda(\mathbb{H})$) such that

$$\sum_{L=0}^{\infty} \mathcal{P}_L\big(\mathbb{H} - \lambda(\mathbb{H})\big)\mathcal{P}_L \;\leqslant\; \mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(2)}) + \widetilde{\kappa_1}\mathcal{N},$$

and hence, by Theorem 3.5, there exists $\kappa_1 > 0$ such that

$$\sum_{L=0}^{\infty} \mathcal{P}_L\big(\mathbb{H} - \lambda(\mathbb{H})\big)\mathcal{P}_L \;\leqslant\; \kappa_1(\mathbb{H} + \kappa_1).$$

The claim is then proven thanks to (3.114).

To prove (3.119) we apply Proposition (3.13) with $A = \widetilde{H}_N^{\mathrm{MF}} - \lambda(\widetilde{H}_N^{\mathrm{MF}})$ and $\sigma = 2$. To compute the A_0 corresponding to $\widetilde{H}_N^{\mathrm{MF}} - \lambda(\widetilde{H}_N^{\mathrm{MF}})$, we first note that Proposition 3.8 implies the existence of $\kappa_3 > 0$ such that $\widetilde{H}_N^{\mathrm{MF}} \leqslant \kappa_3(\mathbb{H} + \kappa_3)$ on $\mathcal{F}_+^{\leqslant M}$ with $M \leqslant N$. Hence,

$$\begin{aligned}\sum_{L=0}^{N} \mathcal{P}_L \widetilde{H}_N^{\mathrm{MF}} \mathcal{P}_L \;&\leqslant\; \kappa_3 \sum_{L=0}^{N} \mathcal{P}_L(\mathbb{H} + \kappa_3)\mathcal{P}_L \\ &\leqslant\; \kappa_3'\big(\mathrm{d}\Gamma^{(1)}(h^{(1)})|_{\mathcal{F}_+^{\leqslant N}} + \mathrm{d}\Gamma^{(2)}(h^{(2)})|_{\mathcal{F}_+^{\leqslant N}} + \kappa_3'\big),\end{aligned} \tag{3.120}$$

where the second inequality is due to (3.49). Now, as a consequence of Assumptions (A_1^{MF}) and (A_2^{MF}), there exist constants $\eta, \tau > 0$ such that the following stability inequality holds

$$H_N^{\mathrm{MF}} \;\geqslant\; \eta\Big(\sum_{i=1}^{N_1} h^{(1)} + \sum_{j=1}^{N_2} h^{(2)}\Big) - \tau N.$$

Through a conjugation by U_N, last estimate can be rewritten as

$$\mathrm{d}\Gamma^{(1)}(h^{(1)}) + \mathrm{d}\Gamma^{(2)}(h^{(2)}) \;\leqslant\; \eta^{-1}\widetilde{H}_N^{\mathrm{MF}} + \eta^{-1}\tau N. \tag{3.121}$$

Combining (3.121) with (3.120), we obtain that there exists $\kappa_2' > 0$ such that

$$\sum_{L=0}^{N} \mathcal{P}_L \widetilde{H}_N^{\mathrm{MF}} \mathcal{P}_L \;\leqslant\; \kappa_2'\big(\widetilde{H}_N^{\mathrm{MF}} + \kappa_2' N\big). \tag{3.122}$$

Moreover, (3.121) also implies the estimate

$$\lambda(\widetilde{H}_N^{\mathrm{MF}}) \;\geqslant\; -\tau N \tag{3.123}$$

The claim then follows from (3.114), because (3.122) and (3.123) imply

$$\sum_{L=0}^{N} \mathcal{P}_L\big(\widetilde{H}_N^{\mathrm{MF}} - \lambda(\widetilde{H}_N^{\mathrm{MF}})\big)\mathcal{P}_L \;\leqslant\; \kappa_2\big(\widetilde{H}_N^{\mathrm{MF}} + \kappa_2 N\big)$$

for a suitable constant κ_2. □

3.5.2 Energy upper bound

We start by proving an upper bound for the ground state energy of the form $\lambda(\widetilde{H}_N^{\mathrm{MF}}) \leqslant \lambda(\mathbb{H}) + o(1)$. Using Lemma 3.118, Proposition 3.8, and the trivial estimate $\mathbb{H} \geqslant \lambda(\mathbb{H})$, we get the following inequality, valid on the space $\mathcal{D}(\mathbb{H}) \cap \mathcal{F}_+^{\leqslant N}$, for $1 \leqslant M \leqslant N$:

$$\mathbb{H} \;\geqslant\; f_M\Big[\Big(1 + C\sqrt{\frac{M}{N}}\Big)^{-1}\widetilde{H}_N^{\mathrm{MF}} - C\sqrt{\frac{M}{N}}\Big] f_M + \lambda(\mathbb{H}) g_M^2 - \frac{\kappa_1}{M^2}(\mathbb{H} + \kappa_1). \tag{3.124}$$

Since, by construction, the function g satisfies $g^2(x) \leqslant 2x$, we have

$$g_M^2 \;\leqslant\; \frac{2\mathcal{N}}{M},$$

and, using the estimate $\mathcal{N} \leqslant C(\mathbb{H}+C)$ which follows from Theorem 3.5, we get

$$\langle g_M^2 \rangle_{\Phi^{\mathrm{gs}}} \;\leqslant\; \frac{C}{M}$$

for some constant C depending on $\lambda(\mathbb{H})$. This implies that, eventually for M and N large enough, $\langle f_M^2 \rangle_{\Phi^{\mathrm{gs}}} > 0$. Hence, after taking the expectation value of (3.124) on Φ^{gs}, we are allowed to divide both sides of the outcome by $\langle f_M^2 \rangle_{\Phi^{\mathrm{gs}}}$ and rearrange terms using $f^2 + g^2 = 1$; what we get is

$$\lambda(\mathbb{H}) \;\geqslant\; \Big(1 + C\sqrt{\frac{M}{N}}\Big)^{-1} \frac{\langle f_M \Phi^{\mathrm{gs}}, \widetilde{H}_N^{\mathrm{MF}} f_M \Phi^{\mathrm{gs}} \rangle}{\langle f_M^2 \rangle_{\Phi^{\mathrm{gs}}}} - C\sqrt{\frac{M}{N}} - \frac{\kappa_1}{M^2 \langle f_M^2 \rangle_{\Phi^{\mathrm{gs}}}} \big(\lambda(\mathbb{H}) + \kappa_1\big). \tag{3.125}$$

Now, in the first summand in the r.h.s. we can exploit the fact that the energy of $f_M \Phi^{\mathrm{gs}}$ is certainly larger than the ground state energy of $\widetilde{H}_N^{\mathrm{MF}}$. For the third summand in the right, in turn, we can use the estimate $1 - C/M \leqslant \langle f_M^2 \rangle_{\Phi^{\mathrm{gs}}} \leqslant 1$. What we obtain is

$$\lambda(\mathbb{H}) \;\geqslant\; \Big(1 + C\sqrt{\frac{M}{N}}\Big)^{-1} \lambda(\widetilde{H}_N^{\mathrm{MF}}) - C\sqrt{\frac{M}{N}} - \frac{C}{M^2},$$

for a large enough $C > 0$. We can optimize last inequality by choosing $M = N^{1/5}$, and this yields the upper bound

$$\lambda(\widetilde{H}_N^{\mathrm{MF}}) \;\leqslant\; \lambda(\mathbb{H}) + C N^{-2/5}. \tag{3.126}$$

3.5.3 Energy lower bound

We now prove the lower bound $\lambda(\widetilde{H}_N^{\mathrm{MF}}) \geqslant \lambda(\mathbb{H}) - o(1)$. Using (3.119), Proposition 3.8, and the trivial estimate $\widetilde{H}_N^{\mathrm{MF}} \geqslant \lambda(\widetilde{H}_N^{\mathrm{MF}})$, we get the inequality

$$\widetilde{H}_N^{\mathrm{MF}} \;\geqslant\; f_M \Big[\Big(1 - C\sqrt{\frac{M}{N}}\Big)\mathbb{H} - C\sqrt{\frac{M}{N}}\Big] f_M + \lambda(\widetilde{H}_N^{\mathrm{MF}}) g_M^2 - \frac{\kappa_2}{M^2}\big(\widetilde{H}_N^{\mathrm{MF}} + \kappa_2 N\big). \tag{3.127}$$

We are going to take the expectation value of last inequality on the ground state Φ_N of $\widetilde{H}_N^{\mathrm{MF}}$ (Φ_N is defined in (3.116)). Hence, by definition, we will have $\langle \widetilde{H}_N^{\mathrm{MF}} \rangle_{\Phi_N} = \lambda(\widetilde{H}_N^{\mathrm{MF}})$.

Moreover, by Theorem 3.2, since $\psi_N^{\mathrm{MF}} = U_N^* \Phi_N$ is a ground state of H_N^{MF}, it exhibits condensation in the sense of (3.22). Such property directly implies that

$$\lim_{N\to\infty} \frac{\langle \mathcal{N} \rangle_{\Phi_N}}{N} \;=\; 0.$$

This, together with the fact that the function g satisfies $g^2(x) \leqslant 2x$, yields

$$\langle g_M^2 \rangle_{\Phi_N} \;\leqslant\; \frac{2\langle \mathcal{N} \rangle_{\Phi_N}}{M} \underset{N\to\infty}{\longrightarrow} 0,$$

provided M is chosen such that $\langle \mathcal{N} \rangle_{\Phi_N} \ll M \ll N$. Last formula implies in particular that, for N large enough and for M in the chosen regime,

$$\langle f_M^2 \rangle_{\Phi_N} \;>\; 0.$$

Hence, after taking the expectation value of (3.127) on Φ_N, we are allowed to divide by $\langle f_M^2\rangle_{\Phi_N}$ and rearrange terms using $f^2+g^2=1$. The result is

$$\begin{aligned}\lambda(\widetilde{H}_N^{\mathrm{MF}}) \;&\geqslant \Big(1-C\sqrt{\frac{M}{N}}\Big)\frac{\langle f_M\Phi_N,\mathbb{H}f_M\Phi_N\rangle}{\langle f_M^2\rangle_{\Phi_N}}\\ &\quad -C\sqrt{\frac{M}{N}}-\frac{\kappa_2}{M^2\langle f_M^2\rangle_{\Phi_N}}\big(\lambda(\widetilde{H}_N^{\mathrm{MF}})+\kappa_2 N\big).\end{aligned} \tag{3.128}$$

Now, $\langle g_M^2\rangle_{\Phi_N}\to 0$ implies $\langle f_M^2\rangle_{\Phi_N}\to 1$, and hence the second summand on the l.h.s. of (3.128) converges to zero. In the first summand in the r.h.s. we can certainly estimate from below the energy of $f_M\Phi_N$ with the ground state energy $\lambda(\mathbb{H})$. Finally, thanks to (3.123) and $\langle f_M^2\rangle_{\Phi_N}\to 1$, the third summand on the right converges to zero if M is chosen such that

$$\max\{\sqrt{N},\langle\mathcal{N}\rangle_{\Phi_N}\}\;\ll\; M\;\ll\; N.$$

By the last three remarks, (3.128) produces

$$\lambda(\widetilde{H}_N^{\mathrm{MF}})\;\geqslant\;\lambda(\mathbb{H})-\delta_N, \tag{3.129}$$

with $\lim_{N\to\infty}\delta_N=0$.

3.5.4 Ground state convergence

As above, let Φ_N be the ground state of $\widetilde{H}_N^{\mathrm{MF}}$. Then, by the estimate $g^2(x)\leqslant 2x$ and the condensation result (3.22), we have

$$\lim_{N\to\infty} g_M\Phi_N \;=\; 0, \tag{3.130}$$

provided we choose M such that $\max\{\sqrt{N},\langle\mathcal{N}\rangle_{\Phi_N}\}\ll M\ll N$. The convergence we want to prove is

$$\lim_{N\to\infty}\Phi_N\;=\;\Phi^{\mathrm{gs}}, \tag{3.131}$$

and, thanks to (3.130), it is proven if we show

$$\lim_{N\to\infty} f_M\Phi_N\;=\;\Phi^{\mathrm{gs}} \tag{3.132}$$

with M in the regime we already fixed.

First, due to the upper and lower bounds proven above, we have

$$\lambda(\mathbb{H})\;\leqslant\;\frac{\langle f_M\Phi_N,\mathbb{H}f_M\Phi_N\rangle}{\langle f_M^2\rangle_{\Phi_N}}\;\leqslant\;\lambda(\widetilde{H}_N^{\mathrm{MF}})+\delta_N\;\leqslant\;\lambda(\mathbb{H})+\delta_N+CN^{-2/5},$$

which, together with $\langle f_M^2\rangle_{\Phi_N}\to 1$, implies

$$\lim_{N\to\infty}\langle f_M\Phi_N,\mathbb{H}f_M\Phi_N\rangle\;=\;\lambda(\mathbb{H}). \tag{3.133}$$

Now, let us decompose $f_M\Phi_N$ into the component along Φ^{gs} and the component along its orthogonal complement, namely

$$f_M\Phi_N\;=\;a_N\Phi^{\mathrm{gs}}+\Phi_N^{\perp},$$

for a coefficient $a_N \in \mathbb{C}$ and a vector $\Phi_N^\perp \in \mathcal{F}_+$ such that $\Phi_N^\perp \perp \Phi^{\mathrm{gs}}$. Then, since Φ^{gs} is an eigenvector of $\mathbb{H}$, we obtain

$$\begin{aligned}\langle f_M\Phi_N, \mathbb{H} f_M \Phi_N\rangle \;&=\; |a_N|^2 \langle \Phi^{\mathrm{gs}}, \mathbb{H}\Phi^{\mathrm{gs}}\rangle + \langle \Phi_N^\perp, \mathbb{H}\Phi_N^\perp\rangle \\ &\geqslant \lambda(\mathbb{H})|a_N|^2 + \inf\sigma(\mathbb{H}_{|\{\Phi^{\mathrm{gs}}\}^\perp})\|\Phi^\perp\|^2 \\ &= \|f_M\Phi_N\|^2\lambda(\mathbb{H}) + \big(\inf\sigma(\mathbb{H}_{|\{\Phi^{\mathrm{gs}}\}^\perp}) - \lambda(\mathbb{H})\big)\|\Phi^\perp\|^2.\end{aligned} \tag{3.134}$$

Due to (3.133) and (3.50), we conclude $\lim_{N\to\infty}\Phi^\perp = 0$, which is equivalent to

$$\lim_{N\to\infty} \|f_M\Phi_N - a_N\Phi^{\mathrm{gs}}\| \;=\; 0.$$

The latter convergence in Fock space norm is equivalent to the convergence in the j,k-th sector, with $j+k\leqslant M$

$$\lim_{N\to\infty}\Big\| a_N^{-1}\big(f_M U_N \psi_N^{\mathrm{gs}}\big)_{jk} - \Phi_{jk}^{\mathrm{gs}}\Big\|_{L^2(\mathbb{R}^3)^{\otimes_{\mathrm{sym}} j}\otimes L^2(\mathbb{R}^3)^{\otimes_{\mathrm{sym}} k}} \;=\; 0. \tag{3.135}$$

Here we have used $|a_N|\to 1$.

Now, since ψ_N^{gs} is the ground state of a Schrödinger operator, thanks to the diamagnetic inequality we can fix its phase so as to have $\psi_N^{\mathrm{gs}} \geqslant 0$ pointwise almost everywhere. Hence, the function $(f_M U_N \psi_N^{\mathrm{gs}})_{jk}$ is non-negative as well, because it is obtained by integrating ψ_N^{gs} against the positive functions u_0 and v_0 (and f_M contributes only by a non-negative multiplicative factor). Since the L^2-convergence in (3.135) implies pointwise convergence a.e., we deduce that a_N must have a limit $e^{\mathrm{i}\theta}$. If we include this global phase factor inside Φ^{gs}, we deduce that

$$\lim_{N\to\infty} f_M\Phi_N \;=\; \Phi^{\mathrm{gs}}, \tag{3.136}$$

which, thanks to (3.130), implies

$$\lim_{N\to\infty} U_N\psi_N^{\mathrm{MF}} \;=\; \Phi^{\mathrm{gs}}. \tag{3.137}$$

By the definition of U_N, the latter is equivalent to the desired convergence (3.20).

Chapter 4

Effective dynamics of condensate mixtures

This Chapter is devoted to the presentation of results on the effective dynamics of mixtures of condensates ruled by the Hamiltonians H_N^{GP} and H_N^{MF}. These topics are based on my works [67] (in collaboration with Michelangeli) and [77].

Recall that, among the main results of Chapters 2 and 3 is the fact that the ground state (and the low-energy states) of a trapped two-species many-body bosonic system exhibits 100% asymptotics Bose-Einstein condensation, both in the mean-field and Gross-Pitaevskii regime. This is in agreement with experiments in which a bosonic mixture, first trapped and then cooled down to ultra-low temperatures, exhibits BEC. From those results, the dynamical problem of *persistence of condensation* along the many-body time evolution naturally emerges. Let us briefly recall the description of the problem, already presented in the Introduction.

Suppose the initial datum for the many-body time evolution is a wave-function $\psi_N \in \mathcal{H}_{N_1,N_2,\mathrm{sym}}$ exhibiting BEC in the sense (1.6) on some orbitals (u,v). This corresponds to having experimentally prepared a trapped two-component condensate. Now, the many-body time evolution is ruled by the linear Schrödinger equation, which reads

$$\begin{cases} \mathrm{i}\partial_t \psi_{N,t} \;=\; H\psi_{N,t} \\ \psi_{N,t}|_{t=0} \;=\; \psi_N, \end{cases} \tag{4.1}$$

and, for a self-adjoint Hamiltonian H that we shall later specialize, the solution is $\psi_{N,t} = e^{-\mathrm{i}tH}\psi_N$.

If the initial configuration ψ_N, which is prepared in a condensed state, corresponds to a stationary state of H (e.g., the ground state), then the dynamics is trivial. More interestingly, one can instead perturb the system before time evolution (typically, by a sudden change or removal of the trap). What is expected, and confirmed by experiments, is that

- $\psi_{N,t}$ exhibits condensation also for $t \in (0,T)$ onto some condensate functions (u_t, v_t),
- and the evolution of (u_t, v_t) is governed by a system of two coupled *non-linear* Schrödinger equations.

The time-scale T is typically long enough for the system to evolve significantly before the condensed phase breaks down.

Reproducing and proving from first principles the phenomenon of persistence of condensation allows to boil down the difficult problem of monitoring the Schrödinger evolution of N particles to the easier one of monitoring the evolution of the two functions (u_t, v_t). The price is the replacement of the many-body linear dynamics (4.1) with a non-linear effective one, the non-linearity naturally emerging from two-body interactions in the form of cubic terms. In shorts, the dynamical problem consists of the completion of the following diagram, assuming the first line holds at $t = 0$:

$$\begin{tikzcd}
\psi_N \arrow[r, "\text{partial trace}"] \arrow[d, "\text{many-body}"', "\textbf{linear}\text{ dynamics}"'] & \gamma^{(1,1)}_{\psi_N} \arrow[r, "N\to\infty"] \arrow[d] & {|u\otimes v\rangle\langle u\otimes v|} \arrow[d, "\textbf{non-linear}", "\text{Schrödinger eq.}"] \\
\psi_{N,t} \arrow[r] & \gamma^{(1,1)}_{\psi_{N,t}} \arrow[r, "N\to\infty"] & {|u_t\otimes v_t\rangle\langle u_t\otimes v_t|.}
\end{tikzcd} \tag{4.2}$$

What non-linear Schrödinger equations have to be expected can be seen by means of several heuristic arguments that can be found in [67, Section 4].

It is worth noting that the results presented in this Chapter prove for the first time the derivation of effective evolution equation for mixtures. The corresponding one-component problem has, in turn, a vast and by now classical literature. We refer to the review [9] and references therein for an overview on the topic.

4.1 Assumptions and main results

The first main result of this Chapter is the completion of the diagram (4.2) in the mean-field regime, that is, the derivation of the effective dynamics generated by the Hamiltonian H_N^{MF} (defined by (1.13) and (1.14)). We shall prove this result in detail in the course of this Chapter. We will also state a similar result for the Gross-Pitaevskii regime, whose proof we will however omit because it would lengthen too much the present thesis.

The effective system of non-linear SchrÃűdinger equation describing the evolution of (u_t, v_t) in the mean-field regime is

$$\begin{aligned}
&\begin{cases}
\mathrm{i}\partial_t u_t &= -\Delta u_t + U^{(1)}_{\mathrm{trap}} u_t + c_1 (V^{(1)} * |u_t|^2) u_t + c_2 (V^{(12)} * |v_t|^2) u_t \\
\mathrm{i}\partial_t v_t &= -\Delta v_t + U^{(2)}_{\mathrm{trap}} v_t + c_2 (V^{(2)} * |v_t|^2) v_t + c_1 (V^{(12)} * |u_t|^2) v_t
\end{cases} \\
&\ u_t|_{t=0} = u \\
&\ v_t|_{t=0} = v.
\end{aligned} \tag{4.3}$$

Let us specify here the main assumptions under which we are able to prove such claim.

(A_1^{MF}) The one-particle Hamiltonians $\mathcal{K}^{(1)} := -\Delta + U^{(1)}_{\mathrm{trap}}$ and $\mathcal{K}^{(2)} := -\Delta + U^{(2)}_{\mathrm{trap}}$ are self-adjoint and semi-bounded below on $L^2(\mathbb{R}^3)$. It is not restrictive to assume both of them to be positive. This implies that the free (kinetic+trapping) part of the Hamiltonian H_N^{MF}, namely

$$H_N^{\mathrm{MF},(0)} := \sum_{j=1}^{N_1} \mathcal{K}_{x_j} + \sum_{k=1}^{N_2} \mathcal{K}_{y_k}, \tag{4.4}$$

is self-adjoint and positive on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, and that the corresponding form domain $\mathcal{D}[H_N^{\mathrm{MF},(0)}]$ is a Hilbert space w.r.t. the scalar product

$$\langle\psi,\chi\rangle_{\mathcal{D}[H_N^{\mathrm{MF},(0)}]} \;=\; \big\langle(\mathbb{1}+H_N^{\mathrm{MF},(0)})^{1/2}\psi,(\mathbb{1}+H_N^{\mathrm{MF},(0)})^{1/2}\chi\big\rangle\,. \tag{4.5}$$

(A_2^{MF}) For $\alpha\in\{1,2,12\}$, the potential $V^{(\alpha)}$ is a real-valued even function satisfying

$$\begin{array}{c} V^{(\alpha)}\in L^{r_\alpha}(\mathbb{R}^3)+L^{s_\alpha}(\mathbb{R}^3)\\ \text{for some } 2\leqslant r_\alpha\leqslant s_\alpha\leqslant+\infty \end{array}\;,\qquad \alpha\in\{1,2,12\}\,. \tag{4.6}$$

(A_3^{MF}) The Hamiltonian H_N^{MF} is self-adjoint and semi-bounded below on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, and $\mathcal{D}[H_N^{\mathrm{MF}}]\subset\mathcal{D}[H_N^{\mathrm{MF},(0)}]$.

(A_4^{MF}) The initial value problem consisting of the system (4.3) with initial data $u\in\mathcal{D}[\mathcal{K}^{(1)}]$ and $v\in\mathcal{D}[\mathcal{K}^{(2)}]$ has a unique global-in-time solution

$$(u_t,v_t)\;\in\;C(\mathbb{R},X)\cap C^1(\mathbb{R},\mathcal{D}[\mathcal{K}^{(1)}]^*\oplus\mathcal{D}[\mathcal{K}^{(1)}]^*) \tag{4.7}$$

where

$$X\;:=\;(\mathcal{D}[\mathcal{K}^{(1)}]\cap L^{\max\{\widehat{r}_1,\widehat{r}_{12}\}}(\mathbb{R}^3))\oplus(\mathcal{D}[\mathcal{K}^{(2)}]\cap L^{\max\{\widehat{r}_2,\widehat{r}_{12}\}}(\mathbb{R}^3)) \tag{4.8}$$

and

$$\frac{1}{r_\alpha}+\frac{1}{\widehat{r}_\alpha}\;=\;\frac{1}{2}\,,\qquad\frac{1}{s_\alpha}+\frac{1}{\widehat{s}_\alpha}\;=\;\frac{1}{2}\,,\qquad\alpha\in\{1,2,12\}\,. \tag{4.9}$$

We remark that assumptions (A_1^{MF})-(A_4^{MF}) above are cast in an "operational" form that is immediately ready to be exploited in our proofs, whereas the precise constraints that they impose on the potentials $U_{\mathrm{trap}}^{(1)},U_{\mathrm{trap}}^{(2)},V^{(1)},V^{(2)},V^{(12)}$ are left in a somewhat implicit form – observe, for instance that a priori conditions (A_3^{MF}) and (A_4^{MF}) select a sub-class of potentials from condition (A_2^{MF}). It is however easy to recognize that (A_1^{MF})-(A_4^{MF}) cover a wide range of practically relevant cases (analogously to what observed already in [44, Section 3.2]), including for example the inter-particle Coulomb interactions $V^{(\alpha)}(x)=c_\alpha|x|^{-1}$, $\alpha\in\{1,2,12\}$ for ordinary one-body Hamiltonians $\mathcal{K}^{(1)}=\mathcal{K}^{(2)}=-\Delta+|x|^2$.

In particular, concerning the non-emptiness of assumption (A_4^{MF}), the global-in-time well-posedness of the non-linear Cauchy problem (4.3) holds for generic (i.e., not too singular) potentials irrespectively of the sign of the interaction: this is due to the fact that the cubic non-linearity is *non-local* (i.e., of convolution form $V*|\varphi|^2$) and hence energy sub-critical, in full analogy to what happens with the usual one-component non-linear Schrödinger equation [17, Corollary 6.1.2].

We can now state the first main result of this Chapter. The statement involves the indicator of condensation $\alpha_{\psi_{N,t}}^{(1,1)}$ associated to the many-body wave-function $\psi_{N,t}\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ and to the condensate wave-function (u_t,v_t) solution to (4.3). Such indicator was already defined in (1.7) as

$$\alpha_{\psi_{N,t}}^{(1,1)}\;=\;1-\big\langle u_t\otimes v_t\,,\,\gamma_{\psi_{N,t}}^{(1,1)}\,u_t\otimes v_t\big\rangle_{L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)}, \tag{4.10}$$

where $\gamma_{\psi_{N,t}}^{(1,1)}$, defined in (1.3), is the reduced density matrix associated to $\psi_{N,t}$.

Theorem 4.1. *Suppose assumptions* (A_1^{MF})-(A_4^{MF}) *above hold true. Consider a wave-function* $\psi_N \in \mathcal{D}[H_N^{\mathrm{MF}}]$ *with* $\|\psi_N\|_{\mathcal{H}_{N_1,N_2,\mathrm{sym}}} = 1$, *and* $(u,v) \in X$ *(the space defined in* (4.8)*) with* $\|u\|_{L^2(\mathbb{R}^3)} = \|v\|_{L^2(\mathbb{R}^3)} = 1$. *Correspondingly, for* $t \in \mathbb{R}$, *let* $\psi_{N,t} := e^{-\mathrm{i}tH_N^{\mathrm{MF}}}\psi_N$ *be the unique solution in* $C(\mathbb{R}, \mathcal{D}[H_N^{\mathrm{MF}}])$ *to the many-body Schrödinger equation*

$$\mathrm{i}\partial_t \psi_{N,t} \;=\; H_N^{\mathrm{MF}} \psi_{N,t}\,, \qquad \psi_{N,t}|_{t=0} \;=\; \psi_N, \tag{4.11}$$

and let (u_t, v_t) *be the unique solution in* $C(\mathbb{R}, X)$ *(the space* (4.7)-(4.8) *of assumption* (A_4^{MF})*) to the initial value problem* (4.3) *with initial condition* (u,v) *at* $t=0$. *Let* $\alpha^{(1,1)}_{\psi_{N,t}}$ *be the quantity defined in* (4.10). *Then there exists a constant* $\kappa > 0$, *such that*

$$\alpha^{(1,1)}_{\psi_{N,t}} \;\leqslant\; \left(\alpha^{(1,1)}_{\psi_N} + \frac{1}{N}\right) e^{\,\kappa f(t)}, \tag{4.12}$$

where

$$\begin{aligned} f(t) \;:=&\; \big\|V^{(1)}\big\|_{L^{r_1}+L^{s_1}} \int_0^t \big(\|u_\tau\|_{\widehat{r}_1} + \|u_\tau\|_{\widehat{s}_1}\big)\,\mathrm{d}\tau \\ &+ \big\|V^{(2)}\big\|_{L^{r_2}+L^{s_2}} \int_0^t \big(\|v_\tau\|_{\widehat{r}_2} + \|v_\tau\|_{\widehat{s}_2}\big)\,\mathrm{d}\tau \\ &+ \big\|V^{(12)}\big\|_{L^{r_{12}}+L^{s_{12}}} \int_0^t \big(\|u_\tau\|_{\widehat{r}_{12}} + \|u_\tau\|_{\widehat{s}_{12}} + \|v_\tau\|_{\widehat{r}_{12}} + \|v_\tau\|_{\widehat{s}_{12}}\big)\,\mathrm{d}\tau. \end{aligned}$$

Theorem 4.1 is proven in Section 4.3.

As anticipated, we are interested in the case in which the initial state ψ_N exhibits condensation in the orbitals u and v. This, together with the estimates of Section 1.2, leads to the following:

Corollary 4.2. *If, in addition to the hypothesis of Theorem 4.1, the initial datum* ψ_N *satisfies*

$$\alpha^{(1,1)}_{\psi_N} \;\leqslant\; \frac{K}{N}\,, \tag{4.13}$$

for some constant $K > 0$, *then* $\forall t \in \mathbb{R}$ *one has*

$$\alpha^{(1,1)}_{\psi_{N,t}} \;\leqslant\; \frac{K+1}{N} e^{\kappa f(t)} \tag{4.14}$$

and also

$$\mathrm{Tr}\,\big|\,\gamma^{(1,1)}_{\psi_{N,t}} - |u_t \otimes v_t\rangle\langle u_t \otimes v_t|\,\big| \;\lesssim\; \frac{e^{\kappa f(t)/2}}{\sqrt{N}}. \tag{4.15}$$

Corollary 4.2 provides therefore a quantitative proof of persistence of double condensation in the mixture at any finite time. Observe that no matter how faster than N^{-1} is the asymptotic BEC (4.13) at $t = 0$, the bound (4.12) always gives at later times a rate of convergence of magnitude N^{-1} in (4.14). We emphasize also that the exponential deterioration in time of all the above controls (4.12), (4.14), (4.15) of BEC along the time evolution is certainly non optimal and is rather a consequence of the Grönwall-type estimate at the basis of the proof of Theorem 4.1.

Remark 4.3 (Control in the energy space). By replacing assumptions (A_2^{MF}) and (A_4^{MF}) above with

($A_2^{\mathrm{MF}}{}'$) The potentials $V^{(\alpha)}$, $\alpha \in \{1,2,12\}$ are real-valued, even, and such that

$$\begin{aligned} \big\|\big(V^{(\alpha)}\big)^2 * |\phi|^2\big\|_\infty &\lesssim \|\phi\|^2_{\mathcal{D}[\mathcal{K}^{(\alpha)}]} \qquad \forall \phi \in \mathcal{D}[\mathcal{K}^{(\alpha)}] \qquad \alpha \in \{1,2\} \\ \big\|\big(V^{(12)}\big)^2 * |\phi|^2\big\|_\infty &\lesssim \|\phi\|^2_{\mathcal{D}[\mathcal{K}^{(\alpha)}]} \qquad \forall \phi \in \mathcal{D}[\mathcal{K}^{(\alpha)}] \qquad \alpha \in \{1,2\}. \end{aligned} \tag{4.16}$$

($A_4^{\mathrm{MF}}{}'$) The initial value problem (4.3) with $u \in \mathcal{D}[\mathcal{K}^{(1)}]$ and $v \in \mathcal{D}[\mathcal{K}^{(2)}]$ has a unique global-in-time solution

$$(u_t, v_t) \;\in\; C(\mathbb{R}, \mathcal{D}[\mathcal{K}^{(1)}] \oplus \mathcal{D}[\mathcal{K}^{(2)}]) \cap C^1(\mathbb{R}, \mathcal{D}[\mathcal{K}^{(1)}]^* \oplus \mathcal{D}[\mathcal{K}^{(2)}]^*), \tag{4.17}$$

Theorem 4.1 and Corollary 4.2 hold with

$$f(t) \;:=\; \int_0^t \Big(\|u_\tau\|^2_{\mathcal{D}[h_1]} + \|v_\tau\|^2_{\mathcal{D}[h_2]}\Big)\,\mathrm{d}\tau.$$

Indeed, assumptions (4.16) take the role of Lemma 4.8 below and the proof remains virtually unchanged.

Remark 4.4 (Persistence of condensation for a fraction of one population). It follows straightforwardly from the properties of the indicators of condensation discussed in Lemma 1.2 of Section 1.2 that the conclusion of Corollary 4.2 implies also

$$\alpha^{(k_1,k_2)}_{\psi_{N,t}} \;\lesssim\; \frac{\max\{k_1,k_2\}}{N}\, e^{\kappa f(t)} \qquad \forall t \in \mathbb{R}, \tag{4.18}$$

which is interpreted as the control of the persistence in time of condensation for up to $o(N_j)$ particles of the j-th species, $j = 1,2$.

Remark 4.5 (More singular potentials). Although we are not interested in discussing in full generality the class of interaction potentials that can be dealt with by the present method, it is worth remarking that with a moderate additional effort one can adapt the proof of Theorem 4.1 (in the spirit of [44, Section 5]) so as to include potentials with stronger singularities than those admitted by Assumptions (A_1^{MF})-(A_4^{MF}) above.

Remark 4.6 (Control of condensation separately in each component). In a similar setting to the one analyzed here, T. Heil [39] has discussed the large N_1, N_2 asymptotics separately for each one-component reduced density matrix, $\gamma^{(1,0)}_{\psi_{N,t}}$ and $\gamma^{(0,1)}_{\psi_{N,t}}$ in our notation. As remarked already, due to the bounds of Lemma 1.1 and Lemma 1.2, such a control is covered by our collective indicator $\gamma^{(1,1)}_{\psi_{N,t}}$.

A result analogous to Theorem 4.1 holds in the Gross-Pitaevskii regime as well. Here, the two-component condensate whose many-body Hamiltonian is H_N^{GP} (defined by (1.13) and (1.14)) has effective dynamics ruled by

$$\begin{aligned} &\begin{cases} \mathrm{i}\partial_t u_t \;=\; -\Delta u_t + c_1 8\pi a_1 |u_t|^2 u_t + c_2 8\pi a_{12} |v_t|^2 u_t \\ \mathrm{i}\partial_t v_t \;=\; -\Delta v_t + c_2 8\pi a_2 |v_t|^2 v_t + c_1 8\pi a_{12} |u_t|^2 v_t \end{cases} \\ &u_t|_{t=0} \;=\; u \\ &v_t|_{t=0} \;=\; v, \end{aligned} \tag{4.19}$$

for suitable (u,v) that we shall specify below. Notice that, for simplicity, we are only discussing the case $U^{(1)}_{\mathrm{trap}} = U^{(2)}_{\mathrm{trap}} = 0$.

The main difference in the treatment of the Gross-Pitaevskii regime is that, not only the many-body initial datum needs to exhibit condensation on (u, v), but it also needs be energetically compatible with $\mathcal{E}^{\mathrm{GP}}[u, v]$ (defined in (1.18)).

We require the following assumptions.

(A_1^{GP}) The external potentials are set to zero, i.e. $U_{\mathrm{trap}}^{(\alpha)} = 0$ for $\alpha \in \{1, 2\}$.

(A_2^{GP}) The potentials $V^{(\alpha)}$, $\alpha \in \{1, 2, 12\}$ are positive, spherically symmetric, compactly supported, L^∞-functions.

(A_3^{GP}) The initial data for the system (4.19) are $u, v \in L^2(\mathbb{R}^3)$ with $\|u\|_2 = \|v\|_2 = 1$ chosen such that the solution (u_t, v_t) belongs to

$$L^\infty\Big(\mathbb{R}, H^2(\mathbb{R}^3) \oplus H^2(\mathbb{R}^3)\Big).$$

(A_4^{GP}) The many-body initial datum is $\psi_N \in \mathcal{D}[H_N^{\mathrm{GP}}] \cap \mathcal{H}_{N_1, N_2, \mathrm{sym}}$ with $\|\psi_N\|_{\mathcal{H}_{N_1,N_2,\mathrm{sym}}} = 1$ and

$$\lim_{N_1, N_2 \to \infty} \gamma_{\psi_N}^{(1,1)} = \ |u \otimes v\rangle\langle u \otimes v|.$$

(A_5^{GP}) The many-body initial datum ψ_N satisfies

$$\lim_{N_1, N_2 \to \infty} \frac{\langle \psi_N, H_N^{\mathrm{GP}} \psi_N \rangle}{N} = \mathcal{E}^{\mathrm{GP}}[u, v].$$

We can now state the main result for the Gross-Pitaevskii regime.

Theorem 4.7. *Consider a two-species bosonic system under assumptions* (A_1^{GP})*-*(A_5^{GP}) *above. Let* $\gamma_{\psi_{N,t}}^{(1,1)}$ *be the reduced density matrix associated with* $\psi_{N,t} = e^{-\mathrm{i}tH_N^{\mathrm{GP}}}\psi_N$. *Then*

$$\lim_{N_1, N_2 \to \infty} \gamma_{\psi_{N,t}}^{(1,1)} = \ |u_t \otimes v_t\rangle\langle u_t \otimes v_t|, \tag{4.20}$$

where (u_t, v_t) *is solves* (4.19).

If the limits in (A_4^{GP}) and (A_5^{GP}) hold with a power-law convergence $N^{-\eta}$ for some $\eta > 0$, then (4.20) holds with a power-law convergence rate $N^{-\eta'}$ for some $\eta' > 0$. However, such convergence is left implicit since highly non-optimal.

Notice that the energy compatibility condition (A_5^{GP}) is trivially propagated along time evolution due to the independence on time of H_N^{GP} and to the conservation of $\mathcal{E}^{\mathrm{GP}}$ along (4.19).

The one-component problem corresponding to Theorem 4.7, namely the derivation of the Gross-Pitaevskii equation

$$\mathrm{i}\partial_t u_t \ = \ -\Delta u_t + 8\pi a |u_t|^2 u_t,$$

has been an important open problem in mathematical physics. It was first solved by Erdős, Schlein and Yau in 2006 [30], [28], [29], [31]; their proof was based on the BBGKY formalism and did not provide a convergence rate. Later results by Benedikter, de Oliveira, and Schlein [8] and by Pickl [82] relied on different techniques and allowed to get a quantitative control of the convergence. The optimal convergence rate was obtained more recently by Brennecke and Schlein [15].

A result analogous to Theorem 4.7 holds in presence of external potentials $U^{(\alpha)}_{\mathrm{trap}}$, $\alpha \in \{1,2\}$. Moreover, a generalization of the technique used in the proof allows to cover the case of the magnetic Laplacian $\Delta_A = (\nabla - iA)^2$. This was pointed out first in [82, Remark 2.1] and then in my work [78], whose main statement is presented in Chapter 5.

The positivity of $V^{(\alpha)}$, $\alpha \in \{1,2,12\}$, assumed in (A_2^{GP}), is the two-component counterpart of the analogous positivity requirement of many previous works in the derivation of the Gross-Pitaevskii equation. This assumption was recently relaxed by Jeblick and Pickl [42] in the one-component context, by replacing it with a stability condition for potentials that might have a small negative part.

The proof of Theorem 4.7, sketched in [77], goes through a suitable adaptation of the one-component result [82]. We shall not report it here.

4.2 Notations and estimates

In this Section we specify an amount of simplified notation that will be used from now on. We also provide some estimates on convolutions that will appear in the proof of Theorem 4.1.

We shall use the convention T^A (resp., T^B) for $T \otimes \mathbb{1}$ (resp., $\mathbb{1} \otimes T$) where T is an operator that acts only on one of the two factors of $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ and we need to consider it as an operator on the whole $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ with trivial action on the other factor. When, in particular, T is a one-particle operator (that is, T acts on $L^2(\mathbb{R}^3)$), the notation T_j^A for some $j \in \{1,\dots,N_1\}$ or T_ℓ^B for some $\ell \in \{1,\dots,N_2\}$ indicates that we are considering T as acting non-trivially on the one-body space of the j-th particle of the first species or the ℓ-th particle of the second species. In the same spirit, we shall write T_{ij} when a *two*-body operator T (i.e., an operator on $L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$, meant to be the one-body spaces of each component) acts on $\mathcal{H}_{N_1,N_2,\mathrm{sym}}$ non-trivially only in the variables x_i and y_j of the wave-function $\psi(x_1,\dots,x_{N_1};y_1,\dots,y_{N_2})$.

A special notation for a number of relevant one-particle operators will be convenient. By h^u and h^v we shall denote the two "one-body non-linear Hamiltonians"

$$\begin{aligned} h^u \; &:= \; \mathcal{K}^{(1)} + c_1 V^{(1)} * |u_t|^2 + c_2 V^{(12)} * |v_t|^2 \\ h^v \; &:= \; \mathcal{K}^{(2)} + c_2 V^{(2)} * |v_t|^2 + c_1 V^{(12)} * |u_t|^2 \end{aligned} \tag{4.21}$$

and by p^A, p^B and q^A, q^B we shall denote the orthogonal projections

$$\begin{aligned} p^A \; &:= \; |u_t\rangle\langle u_t| \,, \qquad & q^A \; &:= \; \mathbb{1} - |u_t\rangle\langle u_t| \\ p^B \; &:= \; |v_t\rangle\langle v_t| \,, \qquad & q^B \; &:= \; \mathbb{1} - |v_t\rangle\langle v_t| \,. \end{aligned} \tag{4.22}$$

Furthermore, we shall make use of the shorthands

$$\begin{aligned} V^{(1),u} \; &:= \; V^{(1)} * |u_t|^2 \,, \qquad & V^{(2),v} \; &:= \; V^{(2)} * |v_t|^2 \\ V^{(12),u} \; &:= \; V^{(12)} * |u_t|^2 \,, \qquad & V^{(12),v} \; &:= \; V^{(12)} * |v_t|^2 \,. \end{aligned} \tag{4.23}$$

Observe that according to our convention $(V^{(1),u})_i^A$ denotes the multiplication operator by the function $(V^{(1)} * |u_t|^2)(x_i)$ in the i-th of the variables for the species A, and so on.

If f^φ is any of the shorthands (4.23) for some functions $f \in \{V^{(1)}, V^{(2)}, V^{(12)}\}$ and $\varphi \in \{u,v\}$, then in terms of the above conventions one has

$$p_2^A f_{12}^A p_2^A \; = \; p_2^A (f^\varphi)_1^A \; = \; p_2^A (f^\varphi)_1^A p_2^A \tag{4.24}$$

as an identity of two-body operators acting on the A-sector of the many-body Hilbert space – here f^A_{12} is the function $f(x_1 - x_2)$ – and the same holds for the B-sector. Analogously,

$$\begin{aligned} p_1^A f_{11}\, p_1^A &= p_1^A (f^\varphi)_1^B = p_1^A (f^\varphi)_1^B p_1^A \\ p_1^B f_{11}\, p_1^B &= p_1^B (f^\varphi)_1^A = p_1^B (f^\varphi)_1^A p_1^B \end{aligned} \tag{4.25}$$

as an identity of mixed-component two-body operators – here f_{11} is the function $f(x_1 - y_1)$.

As we will systematically need to bound the L^∞-norm of functions of the form $V * |\phi|^2$ or $V^2 * |\phi|^2$, where $V = V^{(1)}, V^{(2)}, V^{(12)}$ and $\phi = u_t, v_t$, we cast two standard estimates in the following Lemma.

Lemma 4.8. *For given r, s such that $2 \leqslant r \leqslant s \leqslant \infty$ let $\widehat{r}$ and $\widehat{s}$ be defined by*

$$\frac{1}{r} + \frac{1}{\widehat{r}} = \frac{1}{2}, \qquad \frac{1}{s} + \frac{1}{\widehat{s}} = \frac{1}{2}.$$

Then, for $V \in L^r(\mathbb{R}^d) + L^s(\mathbb{R}^d)$ and $\phi \in L^2(\mathbb{R}^d) \cap L^{\widehat{r}}(\mathbb{R}^d)$ with $\|\phi\|_2 = 1$ one has $\phi \in L^{\widehat{s}}(\mathbb{R}^d)$ and moreover

$$\big\| V * |\phi|^2 \big\|_\infty \leqslant \|V\|_{L^r + L^s} \big(\|\phi\|_{\widehat{r}} + \|\phi\|_{\widehat{s}} \big) \tag{4.26}$$

and

$$\big\| V^2 * |\phi|^2 \big\|_\infty \leqslant 2\, \|V\|^2_{L^r + L^s} \big(\|\phi\|_{\widehat{r}} + \|\phi\|_{\widehat{s}} \big)^2 . \tag{4.27}$$

Proof. By assumption one can split $V = V_r + V_s$ with $V_r \in L^r(\mathbb{R}^d)$ and $V_s \in L^s(\mathbb{R}^d)$, Then

$$\begin{aligned} \big\| V * |\phi|^2 \big\|_\infty &\leqslant \|V_r * |\phi|^2\|_\infty + \|V_s * |\phi|^2\|_\infty \\ &\leqslant \|V_r\|_r \|\phi\|^2_{\frac{2r}{r-1}} + \|V_s\|_s \|\phi\|^2_{\frac{2s}{s-1}} \\ &\leqslant \big(\|V_r\|_r + \|V_s\|_s \big) \big(\|\phi\|^2_{\frac{2r}{r-1}} + \|\phi\|^2_{\frac{2s}{s-1}} \big) \\ &\leqslant \big(\|V_r\|_r + \|V_s\|_s \big) \big(\|\phi\|_{\widehat{r}} + \|\phi\|_{\widehat{s}} \big) \end{aligned}$$

where the second step follows by Young's inequality and the last step by interpolation on $\frac{2r}{r-1} \in [2, \widehat{r}]$ and on $\frac{2s}{s-1} \in [2, \widehat{s}]$, using also the fact that $\|\phi\|_2 = 1$. By taking the infimum over all decompositions of V one obtains

$$\big\| V * |\phi|^2 \big\|_\infty \leqslant \|V\|_{L^r + L^s} \big(\|\phi\|_{\widehat{r}} + \|\phi\|_{\widehat{s}} \big)$$

which proves (4.26). Analogously one finds

$$\begin{aligned} \big\| V^2 * |\phi|^2 \big\|_\infty &\leqslant 2 \big\| V_r^2 * |\phi|^2 \big\|_\infty + 2 \big\| V_s^2 * |\phi|^2 \big\|_\infty \\ &\leqslant 2 \|V_r\|_r^2 \, \|\phi\|^2_{\frac{2r}{r-2}} + 2 \|V_s\|_s^2 \, \|\phi\|^2_{\frac{2s}{s-2}} \\ &\leqslant 2 \big(\|V_r\|_r + \|V_s\|_s \big)^2 \big(\|\phi\|_{\widehat{r}} + \|\phi\|_{\widehat{s}} \big)^2 , \end{aligned}$$

using again Young's inequality in the second step. By taking the infimum over all decompositions of V one obtains

$$\big\| V^2 * |\phi|^2 \big\|_\infty \leqslant 2\, \|V\|^2_{L^r + L^s} \big(\|\phi\|_{\widehat{r}} + \|\phi\|_{\widehat{s}} \big)^2 .$$

which proves (4.27). ∎

4.3 Proof of Theorem 4.1

In this Section we present the proof of Theorem 4.1 and of Corollary 4.2. We shall discuss it in various steps.

The proof goes through a suitable modification of Pickl's counting method for the dynamics of a single-component condensate [44], [83], [81], [82], in order to deal with the inter-species interaction terms and the new mean-field coupling factors. This method is specifically tailored for the quantity $\alpha^{(1,1)}_{\psi_{N,t}}$ and it is designed to control it in terms of its value at $t=0$. In fact, what in an appropriate sense is actually "counted" is, informally speaking, the number of particles of each species in the many-body state $\psi_{\psi_{N,t}}$ which are not of the type u_t or v_t, more precisely which are described by a one-body orbital orthogonal to u_t or v_t. The quantity of interest, according to this interpretation, is therefore the expectation of the observable $|u_t\otimes v_t\rangle\langle u_t\otimes v_t|$ on $L^2(\mathbb{R}^3)\otimes L^2(\mathbb{R}^3)$ on the state $\psi_{N,t}\in\mathcal{H}_{N_1,N_2,\mathrm{sym}}$, and hence the quantity

$$\begin{aligned}\big\langle\psi_{N,t},(\mathbb{1}-|u_t\otimes v_t\rangle\langle u_t\otimes v_t|)\,\psi_{N,t}\big\rangle\;&=\\ =\;1-\big\langle u_t\otimes v_t,\gamma^{(1,1)}_{\psi_{N,t}}\,u_t\otimes v_t\big\rangle\;&=\;\alpha^{(1,1)}_{\psi_{N,t}}.\end{aligned}\tag{4.28}$$

In order to obtain the bound (4.12) in Theorem 4.1 we shall establish the following estimate on the time derivative of $\alpha^{(1,1)}_{\psi_{N,t}}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\alpha^{(1,1)}_{\psi_{N,t}}\;\leqslant\;B(t)\,\alpha^{(1,1)}_{\psi_{N,t}}+\frac{B(t)}{N}\,,\qquad t\in\mathbb{R}\,,\tag{4.29}$$

for some function $B(t)$ that is given in terms of certain norms of the interaction potentials $V^{(1)}$, $V^{(2)}$, $V^{(12)}$ and of the solutions u_t, v_t to the Hartree system, and *independent* of the number of particles. Explicitly,

$$\begin{aligned}B(t)\;&=\kappa\Big(\big\|V^{(1)}\big\|_{L^{r_1}+L^{s_1}}\big(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\big)+\big\|V^{(2)}\big\|_{L^{r_2}+L^{s_2}}\big(\|v\|_{\widehat{r}_2}+\|v\|_{\widehat{s}_2}\big)\\&\qquad+\big\|V^{(12)}\big\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}+\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\Big)\end{aligned}\tag{4.30}$$

for some constant κ that depends only on the population fractions c_1 and c_2.

After an integration in time, (4.29) gives

$$\alpha^{(1,1)}_{\psi_{N,t}}\;\leqslant\;\alpha^{(1,1)}_{\psi_N}+\frac{1}{N}\int_0^t B(s)\,\mathrm{d}s+\int_0^t B(s)\,\alpha^{(1,1)}_{\psi_{N,s}}\,\mathrm{d}s\tag{4.31}$$

which is of the form

$$\alpha(t)\;\leqslant\;\beta(t)+\int_0^t\gamma(s)\,\alpha(s)\,\mathrm{d}s$$

for $\beta(t)\equiv\alpha^{(1,1)}_{\psi_N}+(N)^{-1}\int_0^t B(s)\,\mathrm{d}s$ and $\gamma(t)\equiv B(t)$ and hence implies the Grönwall-like estimate [79, Theorem 1.3.2]

$$\alpha(t)\;\leqslant\;\beta(t)+\int_0^t\beta(s)\,\gamma(s)\,e^{\int_s^t\gamma(r)\,\mathrm{d}r}\,\mathrm{d}s.$$

By further integrations by parts we finally conclude that (4.29) implies

$$\alpha^{(1,1)}_{\psi_{N,t}}\;\leqslant\;\Big(\alpha^{(1,1)}_{\psi_N}+\frac{1}{N}\Big)\,e^{\int_0^t B(s)\,\mathrm{d}s}.\tag{4.32}$$

The bound (4.32), together with (4.30), leads to (4.12). Hence, all is needed is the proof of (4.29).

4.3.1 Time derivative of $\alpha^{(1,1)}_{\psi_{N,t}}$ and cancellation of the kinetic terms

In the following we shall often drop the t-variable and N-subscripts, thus setting $\psi \equiv \psi_N(t)$ for the solution to the many-body Schrödinger equation, $u \equiv u_t$ and $v \equiv v_t$ for the solutions to the Hartree system (4.3) (no confusion should arise with the initial datum (u,v) which will not play a role henceforth). Moreover, we shall often set $\alpha^{(1,1)} \equiv \alpha^{(1,1)}_{\psi_{N,t}}$ and denote its time derivative by $\dot{\alpha}^{(1,1)}$.

We intend to differentiate in time the quantity $\alpha^{(1,1)}$ written in the form (4.28), that is,

$$\alpha^{(1,1)} \;=\; \langle \psi, (\mathbb{1} - p_1^A p_1^B)\psi\rangle \,. \tag{4.33}$$

When the time derivative hits the ψ's, this produces a commutator term $[H_N^{\mathrm{MF}}, p_1^A p_1^B]$ owing to (4.11), and this term is well defined because assumptions (A_2^{MF}) and (A_4^{MF}) imply $p_1^A p_1^B \psi \in \mathcal{D}[H_N^{\mathrm{MF}}]$. When instead the time derivative hits $p_1^A p_1^B$, this produces a commutator term $[(h_1^u)^A + (h_1^v)^B, p_1^A p_1^B]$ owing to (4.3), where h^u and h^v are the operators (4.21). This term too is well defined: indeed, on the one hand Lemma 4.8 together with assumptions (A_2^{MF}) and (A_4^{MF}) implies that the multiplicative parts of h^u and h^v (i.e., the functions $V^{(1)} * |u|^2$, $V^{(2)} * |v|^2$, $V^{(12)} * |u|^2$, and $V^{(12)} * |v|^2$) are all bounded, which in turn implies the boundedness of h^u and h^v as operators $h^u : \mathcal{D}[\mathcal{K}^{(1)}] \to \mathcal{D}[\mathcal{K}^{(1)}]^*$, $h^v : \mathcal{D}[\mathcal{K}^{(2)}] \to \mathcal{D}[\mathcal{K}^{(2)}]^*$; on the other hand $p_1^A p_1^B \psi \in \mathcal{D}[H_N^{\mathrm{MF}}]$ as already observed, and $\mathcal{D}[H_N^{\mathrm{MF}}] \subset \mathcal{D}[H_N^{\mathrm{MF},(0)}]$ owing to assumptions (A_3^{MF}), which makes the expectation $\langle \psi, [(h_1^u)^A + (h_1^v)^B, p_1^A p_1^B]\psi\rangle$ well defined. The conclusion is therefore that $\alpha^{(1,1)}$ is differentiable in time and

$$\dot{\alpha}^{(1,1)} \;=\; \mathrm{i}\,\langle \psi, [H_N^{\mathrm{MF}} - (h_1^u)^A - (h_1^v)^B, \mathbb{1} - p_1^A p_1^B]\,\psi\rangle \,. \tag{4.34}$$

In the r.h.s. of (4.34) the insertion of further terms $(h_j^u)^A$ and $(h_j^v)^B$ with $j \geqslant 2$ does not produce any effect, since their commutator with $\mathbb{1} - p_1^A\, p_1^B$ vanishes. This gives

$$\dot{\alpha}^{(1,1)} \;=\; \mathrm{i}\,\langle \psi, [H_N^{\mathrm{MF}} - (H^u)^A - (H^v)^B, \mathbb{1} - p_1^A p_1^B]\,\psi\rangle \,. \tag{4.35}$$

where

$$H^u \;:=\; \sum_{k=1}^{N_1} h_k^u \,, \qquad H^v := \sum_{\ell=1}^{N_2} h_\ell^v \,. \tag{4.36}$$

Further, one can re-write the r.h.s. of (4.35) as the expectation of an operator that is completely symmetric in each component, namely

$$\dot{\alpha}^{(1,1)} \;=\; \mathrm{i}\,\Big\langle \psi\,, \Big[H_N^{\mathrm{MF}} - (H^u)^A - (H^v)^B\,, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} \frac{\mathbb{1} - p_k^A\, p_\ell^B}{N_1 N_2}\,\Big]\,\psi\Big\rangle \,. \tag{4.37}$$

Observe that when passing from (4.34) to (4.35) one obtains a complete *cancellation of the kinetic* *terms* which will play no role henceforth. Thus,

$$
\begin{aligned}
\dot{\alpha}^{(1,1)} \;=\; \mathrm{i}\Big\langle\psi\,,\Big[\,\frac{1}{N}\sum_{i<j}^{N}(V^{(1)}(x_i-x_j))^A+\frac{1}{N}\sum_{r<s}^{N_2}(V^{(2)}(y_r-y_s)^B \\
&+\frac{1}{N}\sum_{i=1}^{N_1}\sum_{r=1}^{N_2}V^{(12)}(x_i-y_r) \\
&-c_1\sum_{i=1}^{N_1}(V^{(1),u})_i^A-c_2\sum_{i=1}^{N_1}(V^{(12),v})_i^A \\
&-c_2\sum_{r=1}^{N_2}(V^{(2),v})_r^B-c_1\sum_{r=1}^{N_2}(V^{(12),u})_r^B\,,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{\mathbb{1}-p_k^A\,p_\ell^B}{N_1N_2}\,\Big]\,\psi\Big\rangle
\end{aligned}
\tag{4.38}
$$

where we used the shorthands (4.23).

We separate the contributions given to $\dot{\alpha}^{(1,1)}$ by each potential $V^{(1)}$, $V^{(2)}$, $V^{(12)}$ and write

$$
\dot{\alpha}^{(1,1)} \;=\; \mathrm{i}\,(C_{V^{(1)}}+C_{V^{(2)}}+C_{V^{(12)}}) \tag{4.39}
$$

with

$$
C_{V^{(1)}}:=\Big\langle\psi,\Big[\Big(\frac{1}{N}\sum_{i<j}^{N_1}V^{(1)}(x_i-x_j)-c_1\sum_{i=1}^{N_1}(V^{(1),u})_i\Big)^A,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{\mathbb{1}-p_k^A\,p_\ell^B}{N_1N_2}\Big]\psi\Big\rangle, \tag{4.40}
$$

$$
C_{V^{(2)}}:=\Big\langle\psi,\Big[\Big(\frac{1}{N}\sum_{r<s}^{N_2}V^{(2)}(y_r-y_s)-c_2\sum_{r=1}^{N_2}(V^{(2),v})_r\Big)^B,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{\mathbb{1}-p_k^A\,p_\ell^B}{N_1N_2}\Big]\psi\Big\rangle, \tag{4.41}
$$

$$
\begin{aligned}
C_{V^{(12)}}=\Big\langle\psi,\Big[\frac{1}{N}\sum_{i=1}^{N_1}\sum_{r=1}^{N_2}V^{(12)}(x_i-y_r)-c_2\sum_{i=1}^{N_1}(V^{(12),v})_i^A \\
-c_1\sum_{r=1}^{N_2}(V^{(12),u})_r^B,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{\mathbb{1}-p_k^A\,p_\ell^B}{N_1N_2}\Big]\psi\Big\rangle\,.
\end{aligned}
\tag{4.42}
$$

In the following Subsections we shall estimate separately these three terms, see Propositions 4.9 and 4.10 below. The final result, obtained by plugging (4.46) and (4.53) into (4.39), is

$$
\begin{aligned}
\dot{\alpha}^{(1,1)} \;\leqslant\; \kappa\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)\times \\
\times\Big(\|V^{(1)}\|_{L^{r_1}+L^{s_1}}\,\big(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\big)+\|V^{(2)}\|_{L^{r_2}+L^{s_2}}\,\big(\|v\|_{\widehat{r}_2}+\|v\|_{\widehat{s}_2}\big) \\
+\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}+\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\Big)
\end{aligned}
\tag{4.43}
$$

for some constant κ that depends only on the population fractions c_1 and c_2. Formula (4.43) proves (4.29) which, as argued at the beginning of this Section, yields the proof of (4.12).

4.3.2 Terms containing $V^{(1)}$ and $V^{(2)}$

By means of straightforward commutation properties we re-write (4.40) as

$$\begin{aligned} C_{V^{(1)}} &= \Big\langle\psi, \Big[\Big(\frac{1}{N}\sum_{i<j}^{N_1} V^{(1)}(x_i-x_j) - c_1\sum_{i=1}^{N_1}(V^{(1),u})_i\Big)^A, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{-p_k^A\,p_\ell^B}{N_1N_2}\Big]\psi\Big\rangle \\ &= \Big\langle\psi, \Big[\frac{1}{N}\sum_{i<j}^{N_1} V^{(1)}(x_i-x_j) - c_1\sum_{i=1}^{N_1}(V^{(1),u})_i, \sum_{k=1}^{N_1}\frac{-p_k}{N_1}\Big]^A p_1^B\,\psi\Big\rangle \\ &= \Big\langle\psi, \Big[\frac{1}{N}\sum_{i<j}^{N_1} V^{(1)}(x_i-x_j) - c_1\sum_{i=1}^{N_1}(V^{(1),u})_i\,,\,\widehat{m}\Big]^A p_1^B\,\psi\Big\rangle \\ &= \frac{c_1}{2}\big\langle\psi, \big[(N_1-1)(V^{(1)})_{12} - N_1(V^{(1),u})_1 - N_1(V^{(1),u})_2\,,\,\widehat{m}\big]^A p_1^B\,\psi\big\rangle \end{aligned} \tag{4.44}$$

where $\widehat{m}$ is the auxiliary operator defined in (4.69) and (4.72) of the next Section, and where in the third step we applied property (4.73) for $\widehat{m}$ and in the last step we exploited the symmetry of ψ. Analogously, from (4.41),

$$C_{V^{(2)}} = \frac{c_2}{2}\big\langle\psi, \big[(N_2-1)(V^{(2)})_{12} - N_2(V^{(2),v})_1 - N_2(V^{(2),v})_2\,,\,\widehat{m}\big]^B p_1^A\,\psi\big\rangle\,. \tag{4.45}$$

Proposition 4.9. *Under the hypotheses of Theorem 4.1,*

$$\begin{aligned} |C_{V^{(1)}}| &\leqslant \kappa_1\Big(\alpha^{(1,1)} + \frac{1}{N}\Big)\,\|V^{(1)}\|_{L^{r_1}+L^{s_1}}\,\big(\|u\|_{\widehat{r}_1} + \|u\|_{\widehat{s}_1}\big) \\ |C_{V^{(2)}}| &\leqslant \kappa_2\Big(\alpha^{(1,1)} + \frac{1}{N}\Big)\,\|V^{(2)}\|_{L^{r_2}+L^{s_2}}\,\big(\|v\|_{\widehat{r}_2} + \|v\|_{\widehat{s}_2}\big)\,. \end{aligned} \tag{4.46}$$

For both $j=1,2$ the constant κ_j depends only on the population fraction c_j.

Proof. We shall focus on $C_{V^{(1)}}$, the proof for $C_{V^{(2)}}$ is completely analogous. In fact, since the commutator in the r.h.s. of (4.44) is non-trivial on the first component only, the treatment of $C_{V^{(1)}}$ is analogous to the single-component case. By inserting on both sides of the commutator in (4.44) the identity

$$\mathbb{1}^A = (p_1^A + q_1^A)(p_1^A + q_2^A) \tag{4.47}$$

one obtains 16 terms; however, owing to Lemma 4.13, only those terms with different numbers of q's on the left and on the right are non-zero (see the remark after (4.81)). We cast them in the following self-explanatory notation

$$C_{V^{(1)}} = 2\,(pp,qp) + 2\,(qp,qq) + (pp,qq) + \text{complex conjugate} \tag{4.48}$$

We shall estimate each summand above in terms of $\alpha^{(1,1)}$ and $(N)^{-1}$.

The first term is

$$\begin{aligned} (pp,qp) &= \frac{\mathrm{i}c_1}{2}\big\langle\psi, p_1^Ap_2^A\,\Big[(N_1-1)(V^{(1)})_{12} - N_1\,(V^{(1),u})_1, \widehat{m}\Big]^A\,q_1^Ap_2^Ap_1^B\psi\big\rangle \\ &= \frac{\mathrm{i}c_1}{2}\big\langle\psi, p_1^Ap_2^A\,\Big[(N_1-1)(V_1^u)_1 - N_1\,(V^{(1),u})_1, \widehat{m}\Big]^A\,q_1^Ap_2^Ap_1^B\psi\big\rangle \\ &= -\frac{\mathrm{i}c_1}{2}\big\langle\psi, p_1^Ap_2^A\,\Big[\,(V^{(1),u})_1, \widehat{m}\,\Big]^A\,q_1^Ap_2^Ap_1^B\psi\big\rangle \\ &= -\frac{\mathrm{i}c_1}{2N_1}\big\langle\psi, p_1^Ap_2^A(V^{(1),u})_1^A q_1^Ap_2^Ap_1^B\psi\big\rangle\,. \end{aligned}$$

where we used $p_1^A q_1^A = 0$ in the first and last identities and property (4.24) in the second identity. Therefore, by Lemma 4.8,

$$|(pp,qp)| \leqslant \frac{c_1}{2N_1}\|V_1 * |u|^2\|_\infty \leqslant \frac{1}{N}\|V^{(1)}\|_{L^{r_1}+L^{s_1}}\left(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\right). \tag{4.49}$$

Following analogous steps, the second summand in (4.48) becomes

$$\begin{aligned}(qp,qq) &= \frac{\mathrm{i}c_1}{2}\langle\psi, q_1^A p_2^A[(N_1-1)(V_1)_{12} - N_1(V^{(1),u})_2,\widehat{m}\,]^A q_1^A q_2^A p_1^B\psi\rangle \\ &= \frac{\mathrm{i}c_1}{2}\Big\langle\psi, q_1^A p_2^A\Big(\frac{N_1-1}{N_1}(V^{(1)})_{12} - (V^{(1),u})_2\Big)^A q_1^A q_2^A p_1^B\psi\Big\rangle\,.\end{aligned}$$

Splitting the difference we obtain two terms: the second is controlled by a Cauchy-Schwarz inequality and by estimate (4.26) of Lemma 4.8 as

$$\begin{aligned}\frac{1}{2}|\langle\psi, q_1^A p_2^A(V^{(1),u})_2^A q_1^A q_2^A p_1^B\psi\rangle| &\leqslant \frac{1}{2}\,\|V^{(1)} * |u|^2\|_\infty\,\|q_1^A\psi\|^2 \\ &\leqslant \frac{1}{2}\,\|V^{(1)}\|_{L^{r_1}+L^{s_1}}\left(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\right)\alpha^{(1,1)},\end{aligned}$$

having bounded $\|q_1^A\psi\|^2 = \alpha^{(1,0)}$ with $\alpha^{(1,1)}$ (Lemma 1.1). The first term is again controlled by Cauchy-Schwarz as

$$\begin{aligned}&\frac{1}{2}|\langle\psi, q_1^A p_2^A(V^{(1)})_{12}^A\, q_1^A q_2^A p_1^B\psi\rangle| \\ &\qquad\leqslant \frac{1}{2}\sqrt{\langle\psi, q_1^A p_2^A((V^{(1)})_{12}^2)^A\, p_2^A q_1^A\psi\rangle}\,\sqrt{\langle\psi, q_1^A q_2^A p_1^B\psi\rangle} \\ &\qquad= \frac{1}{2}\sqrt{\langle\psi, q_1^A p_2^A(\big(V^{(1)}\big)^2 * |u|^2)_1^A p_2^A q_1^A\psi\rangle}\,\sqrt{\langle\psi, q_1^A q_2^A p_1^B\psi\rangle} \\ &\qquad\leqslant \frac{1}{2}\sqrt{\|\big(V^{(1)}\big)^2 * |u|^2\|_\infty}\,\|q_1^A\psi\|\,\|q_2^A\psi\| \\ &\qquad= \frac{1}{2}\sqrt{\Big\|\big(V^{(1)}\big)^2 * |u|^2\Big\|_\infty}\,\alpha^{(1,1)}\end{aligned}$$

having used Lemma 1.1 in the last step. Then, owing to estimate (4.27) of Lemma 4.8,

$$\frac{1}{2}|\langle\psi, q_1^A p_2^A(V^{(1)})_{12}^A\, q_1^A q_2^A p_1^B\psi\rangle| \leqslant \frac{1}{\sqrt{2}}\,\|V^{(1)}\|_{L^{r_1}+L^{s_1}}\left(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\right)\alpha^{(1,1)}$$

and the conclusion is

$$|(qp,qq)| \lesssim \|V^{(1)}\|_{L^{r_1}+L^{s_1}}\left(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\right)\alpha(1,1)\,. \tag{4.50}$$

The third summand in (4.48) reads

$$\begin{aligned}(pp,qq) &= \frac{\mathrm{i}c_1}{2}\langle\psi, p_1^A p_2^A[(N_1-1)(V^{(1)})_{12},\widehat{m}\,]^A q_1^A q_2^A p_1^B\psi\rangle \\ &= \mathrm{i}c_1\,\frac{N_1-1}{N_1}\langle\psi, p_1^A p_2^A(V^{(1)})_{12}^A\,\widehat{n}^A(\widehat{n}^{-1})^A q_1^A q_2^A p_1^B\psi\rangle \\ &= \mathrm{i}c_1\,\frac{N_1-1}{N_1}\langle\psi, p_1^A p_2^A\,\widehat{\tau_2 n}^A(V^{(1)})_{12}^A(\widehat{n}^{-1})^A q_1^A q_2^A p_1^B\psi\rangle\,,\end{aligned}$$

where in the second step we applied Lemma (4.13) and we introduced the auxiliary operator $\widehat{n}$ defined in (4.69) and (4.71), using the fact that $(\widehat{n}^{-1})^A$ is well defined on the range of q_1^A since $(\widehat{n}^{-1})^A q_1^A\psi = \sum_{k=1}^N (N/k)^{1/2} P_k q_1 \psi$, while the last identity follows from Lemma 4.13 in the form (4.81). Then

$$
\begin{aligned}
|(pp,qq)| \;&\leqslant\; c_1 \sqrt{\langle \psi, p_1^A p_2^A \widehat{\tau_2 n}^A ((V^{(1)})^2_{12})^A \,\widehat{\tau_2 n}^A p_1^A p_2^A \psi\rangle}\sqrt{\langle \psi, (\widehat{n}^{-2})^A q_1^A q_2^A p_1^B \psi\rangle} \\
&\leqslant\; c_1 \sqrt{\langle \psi, p_1^A p_2^A \,\widehat{\tau_2 n}^A (\big(V^{(1)}\big)^2 * |u|^2)_1^A \,\widehat{\tau_2 n}^A p_1^A p_2^A \psi\rangle}\,\sqrt{\frac{N_1}{N_1-1}}\,\|q_2^A\,\psi\| \\
&\leqslant\; 2\,c_1 \sqrt{\|\big(V^{(1)}\big)^2 * |u|^2\|_\infty}\;\big\|\widehat{\tau_2 n}^A \psi\big\|\,\sqrt{\alpha^{(1,1)}} \\
&=\; 2\,c_1 \sqrt{\|\big(V^{(1)}\big)^2 * |u|^2\|_\infty}\;\sqrt{\alpha^{(1,1)}+\frac{2}{N_1}}\;\sqrt{\alpha^{(1,1)}} \\
&\leqslant\; 4\sqrt{\|\big(V^{(1)}\big)^2 * |u|^2\|_\infty}\;\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)
\end{aligned}
$$

where we used the Cauchy-Schwarz inequality in the first step, (4.24) and (4.77) of Lemma 4.12 in the second, the control $\alpha^{(1,0)} \leqslant \alpha^{(1,1)}$ (Lemma 1.1) in the third, (4.69), (4.71), and (4.79) in the fourth, and

$$
\begin{aligned}
\sqrt{\alpha^{(1,1)}+\frac{2}{N_1}}\,\sqrt{\alpha^{(1,1)}} \;&\leqslant\; \alpha^{(1,1)}+\frac{1}{N_1} \;\leqslant\; \frac{N}{N_1}\Big(\alpha^{(1,1)}+\frac{1}{N}\Big) \\
&\leqslant\; \frac{2}{c_1}\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)
\end{aligned}
$$

in the last, for N_1, N_2 sufficiently large. Then, owing to estimate (4.27) of Lemma 4.8 we conclude

$$
|(pp,qq)| \;\leqslant\; 4\sqrt{2}\,\|V^{(1)}\|_{L^{r_1}+L^{s_1}}\,\big(\|u\|_{\widehat{r}_1}+\|u\|_{\widehat{s}_1}\big)\left(\alpha^{(1,1)}+\frac{1}{N}\right). \tag{4.51}
$$

Plugging (4.49), (4.50), and (4.51) into (4.48) yields finally (4.46). □

4.3.3 Term containing $V^{(12)}$

We first write, using the symmetry of ψ:

$$
\begin{aligned}
|C_{V^{(12)}}| \;&\leqslant\; \frac{N_1N_2}{N}\times \\
&\quad\times\Big|\Big\langle\psi,\Big[(V^{(12)})_{11}-(V^{(12),v})_1^A-(V^{(12),u})_1^B,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{p_k^A\,p_\ell^B}{N_1N_2}\Big]\psi\Big\rangle\Big|.
\end{aligned} \tag{4.52}
$$

For the estimate of $C_{V^{(12)}}$ we shall establish the following:

Proposition 4.10. *Under the hypotheses of Theorem 4.1,*

$$
\begin{aligned}
|C_{V^{(12)}}| \;&\leqslant\; \kappa_{12}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}+\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\times \\
&\quad\times\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)
\end{aligned} \tag{4.53}
$$

where the constant κ_{12} depends only on the population fractions c_1 and c_2.

Proof. We insert on both sides of the commutator in (4.52) the identity

$$\mathbb{1} \;=\; (p_1^A + q_1^A)(p_1^B + q_1^B) \tag{4.54}$$

(observe that, as opposite to (4.47), in (4.54) the insertion involves *both* components), which produces 16 terms to estimate. Unlike our previous bookkeeping (4.48), it is not possible to apply Lemma 4.13 in order to identify a priori those terms that vanish, because here the p's and q's inserted on the left and on the right are relative to *distinct* components. We rather group these terms depending on whether the number of the q's is the same or not on both sides, that is,

$$\begin{aligned}\Lambda \;:=\; & (pp,pp) + [(pq,pq) + (qp,qp)] + (qq,qq) \\ & + [(pq,qp) + \text{complex conjugate}\,]\end{aligned} \tag{4.55}$$

and

$$\begin{aligned}\Omega \;:=\; & (pp,qp) + (qp,qq) + (pp,qq) + (pp,pq) + (pq,qq) \\ & +\; \text{complex conjugate}\end{aligned} \tag{4.56}$$

where a self-explanatory notation analogous to (4.48) is used. In the following Subsections we shall prove that

$$|\Lambda| \;\lesssim\; \|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}} + \|u\|_{\widehat{s}_{12}} + \|v\|_{\widehat{r}_{12}} + \|v\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)} \tag{4.57}$$

(see (4.61) below) and

$$\begin{aligned}|\Omega| \;\leqslant\; & \widetilde{\kappa}_{12}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}} + \|u\|_{\widehat{s}_{12}} + \|v\|_{\widehat{r}_{12}} + \|v\|_{\widehat{s}_{12}}\big)\,\times \\ & \times\Big(\alpha^{(1,1)} + \frac{1}{N}\Big)\,.\end{aligned} \tag{4.58}$$

(see (4.64) below), for some constant $\widetilde{\kappa}_{12}$ that depends on c_1 and c_2 only. This completes the proof. □

Terms with the same number of q's on the left and on the right

In order to apply a number of straightforward symmetry and permutation arguments it will be convenient to re-write systematically

$$\Big[A_{11}\,,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} p_k^A\,p_\ell^B\Big] \;=\; \Big[A_{11}\,,\sum_{k=1}^{N_1} p_k^A\,p_1^B + \sum_{\ell=1}^{N_2} p_1^A\,p_\ell^B - p_1^A p_1^B\Big] \tag{4.59}$$

whenever we deal with an observable A_{11} acting on the first variable of each component.

The summand (pp,pp) in (4.55) vanishes because

$$\begin{aligned}&\Big\langle\psi, p_1^A p_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} p_k^A\,p_\ell^B\Big]p_1^A p_1^B\psi\Big\rangle \\ &= \Big\langle\psi, p_1^A p_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B\,, \sum_{k=1}^{N_1} p_k^A\,p_1^B + \sum_{\ell=1}^{N_2} p_1^A\,p_\ell^B - p_1^A p_1^B\Big]p_1^A p_1^B\psi\Big\rangle \\ &=\; 0\end{aligned}$$

where in the first identity we used (4.59) and in the second one we used the fact that the p_1-operators inside the commutator can be re-absorbed in the corresponding p_1's outside, thus yielding a vanishing commutator.

The summand (pq, pq) in (4.55) vanishes because

$$\begin{aligned}
&\Big\langle\psi, p_1^A q_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} p_k^A\, p_\ell^B\Big] p_1^A q_1^B \psi\Big\rangle \\
&= \Big\langle\psi, p_1^A q_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B\,, \sum_{k=1}^{N_1} p_k^A\, p_1^B + \sum_{\ell=1}^{N_2} p_1^A\, p_\ell^B - p_1^A p_1^B\Big] p_1^A q_1^B \psi\Big\rangle \\
&= \Big\langle\psi, p_1^A q_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B\,, \sum_{\ell=2}^{N_2} p_\ell^B\Big] q_1^B \psi\Big\rangle \;=\; 0
\end{aligned}$$

where in the first identity we used (4.59), in the second identity we used $p_1^B q_1^B = \mathbb{O}$ and we re-absorbed p_1^A outside the commutator, and in the last one we used the fact that the two entries of the commutator act on different variables. Obviously, the summand (qp, qp) in (4.55) vanishes for the same reason, upon exchanging the roles of A and B.

The summand (qq, qq) in (4.55) vanishes owing to $pq = \mathbb{O}$, indeed

$$\Big\langle\psi, q_1^A q_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B\,, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} p_k^A\, p_\ell^B\Big] q_1^A q_1^B \psi\Big\rangle \;=\; 0\,,$$

Thus, in order to estimate the quantity Λ in (4.55) it only remains to give a bound to the term of type (pq, qp). One has

$$\begin{aligned}
&\frac{N_1 N_2}{N}\Big\langle\psi, p_1^A q_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} \frac{p_k^A\, p_\ell^B}{N_1 N_2}\Big] q_1^A p_1^B \psi\Big\rangle \\
&= \frac{1}{N}\Big\langle\psi, p_1^A q_1^B\Big[(V^{(12)})_{11}\,, \sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2} p_k^A\, p_\ell^B\Big] q_1^A p_1^B \psi\Big\rangle \\
&= \frac{1}{N}\Big\langle\psi, p_1^A q_1^B\Big[(V^{(12)})_{11}\,, \sum_{k=1}^{N_1} p_k^A\, p_1^B + \sum_{\ell=1}^{N_2} p_1^A\, p_\ell^B\Big] q_1^A p_1^B \psi\Big\rangle \\
&= \frac{N_1 - 1}{N}\big\langle\psi, p_1^A q_1^B (V^{(12)})_{11} p_2^A q_1^A p_1^B \psi\big\rangle - \frac{N_2 - 1}{N}\big\langle\psi, p_1^A q_1^B p_2^B (V^{(12)})_{11} q_1^A p_1^B \psi\big\rangle
\end{aligned}$$

where in the first identity the summand $(V^{(12),v})_1^A$ (respectively $(V^{(12),u})_1^B$) does not contribute because p_1^B (resp., q_1^A) from the right can be pulled through the commutator all the way to the left with $q_1^B p_1^B = \mathbb{O}$ (resp., $p_1^A q_1^A = \mathbb{O}$), in the second identity we used (4.59) and again $pq = \mathbb{O}$, and in the last identity we used the fact that one term of each commutator vanishes because of $pq = \mathbb{O}$.

Therefore, since $(N_j - 1)(N)^{-1} \leqslant c_j \leqslant 1$, $j = 1, 2$,

$$|\Lambda| \;\leqslant\; \big|\big\langle\psi, p_1^A q_1^B (V^{(12)})_{11} p_2^A q_1^A p_1^B \psi\big\rangle\big| + \big|\big\langle\psi, p_1^A q_1^B p_2^B (V^{(12)})_{11} q_1^A p_1^B \psi\big\rangle\big|\,. \tag{4.60}$$

For the first summand in the r.h.s. of (4.60) one has

$$\begin{aligned}\big|\langle\psi,p_1^Aq_1^B(V^{(12)})_{11}p_2^Aq_1^Ap_1^B\psi\rangle\big| \;&\leqslant\; \|(V^{(12)})_{11}p_1^Aq_1^B\psi\|\,\|q_1^Ap_2^Ap_1^B\psi\| \\ &\leqslant\; \sqrt{\langle\psi,p_1^Aq_1^B(V_{12}^2)_{11}p_1^Aq_1^B\psi\rangle}\,\sqrt{\langle\psi,q_1^A\,\psi\rangle} \\ &=\; \sqrt{\langle\psi,p_1^Aq_1^B(V_{12}^2*|u|^2)_1^Bp_1^Aq_1^B\psi\rangle}\,\|q_1^A\psi\| \\ &\leqslant\; \sqrt{\|V_{12}^2*|u|^2\|_\infty}\,\|q_1^B\psi\|\,\|q_1^A\psi\| \\ &\leqslant\; \sqrt{2}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\end{aligned}$$

where we used the Cauchy-Schwarz inequality in the first step, the operator bound $\mathbb{O}\leqslant p\leqslant\mathbb{1}$ in the second and fourth step, identity (4.25) in the third step, and the identities $\alpha^{(1,0)}=\|q_1^A\psi\|^2$ and $\alpha^{(0,1)}=\|q_1^B\psi\|^2$ in the fourth step together with the bounds (1.9) of Lemma 1.1 that produce $\alpha^{(1,1)}$. Along the same line, the second summand in the r.h.s. of (4.60) is estimated as

$$\big|\langle\psi,p_1^Aq_1^Bp_2^B(V^{(12)})_{11}q_1^Ap_1^B\psi\rangle\big| \;\leqslant\; \sqrt{2}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\,.$$

The conclusion is

$$|\Lambda| \;\lesssim\; \|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\,. \tag{4.61}$$

Terms with a different number of q's on the left and on the right

We first check that the terms (pp,qp) and (pp,pq) in (4.56) are zero. Indeed,

$$\begin{aligned}&\Big\langle\psi,\,p_1^Ap_1^B\Big[(V^{(12)})_{11}-(V^{(12),v})_1^A-(V^{(12),u})_1^B\,,\,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}p_k^A\,p_\ell^B\,\Big]q_1^Ap_1^B\psi\Big\rangle \\ &\qquad=\;\Big\langle\psi,p_1^Ap_1^B\Big[(V^{(12)})_{11}-(V^{(12),v})_1^A\,,\,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}p_k^A\,p_\ell^B\,\Big]q_1^Ap_1^B\psi\Big\rangle \\ &\qquad=\;\Big\langle\psi,p_1^Ap_1^B\Big[((V^{(12),v})_1^A-(V^{(12),v})_1^A\,,\,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}p_k^A\,p_\ell^B\,\Big]q_1^Ap_1^B\psi\Big\rangle \;=\;0\,,\end{aligned}$$

where in the first identity the term $(V^{(12),u})_1^B$ does not contribute because q_1^A from the right can be pulled through the commutator all the way to the left with $p_1^Aq_1^A=\mathbb{O}$, and in the second identity we applied (4.25). This shows that $(pp,qp)=0$ and an analogous argument shows that $(pp,pq)=0$.

For the term (qp,qq) in (4.56) one has

$$\begin{aligned}&\frac{N_1N_2}{N}\,\Big\langle\psi,q_1^Ap_1^B\Big[(V^{(12)})_{11}-(V^{(12),v})_1^A-(V^{(12),u})_1^B\,,\,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{p_k^A\,p_\ell^B}{N_1N_2}\,\Big]q_1^Aq_1^B\psi\Big\rangle \\ &=\;\frac{1}{N}\,\Big\langle\psi,q_1^Ap_1^B\Big[(V^{(12)})_{11}-(V^{(12),u})_1^B\,,\,\sum_{k=1}^{N_1}p_k^A\,p_1^B+\sum_{\ell=1}^{N_2}p_1^A\,p_\ell^B-p_1^Ap_1^B\,\Big]q_1^Aq_1^B\psi\Big\rangle \\ &=\;\frac{1}{N}\,\Big\langle\psi,q_1^Ap_1^B\Big[(V^{(12)})_{11}-(V^{(12),u})_1^B\,,\,\sum_{k=2}^{N_1}p_k^A\,p_1^B\,\Big]q_1^Aq_1^B\psi\Big\rangle \\ &=\;-\frac{(N_1-1)}{N}\,\Big\langle\psi,q_1^Ap_1^B\big((V^{(12)})_{11}-(V^{(12),u})_1^B\big)\,q_1^Aq_1^Bp_2^A\,\psi\Big\rangle\,,\end{aligned}$$

where in the first identity we applied (4.59) and we dropped the $(V^{(12),v})_1^A$-term owing to the commutation of q_1^B from the right all the way through to the left with $p_1^B q_1^B = \mathbb{O}$, in the second identity we used $p_1^A q_1^A = \mathbb{O}$, and in the third we used the symmetry of ψ and again $p_1^B q_1^B = \mathbb{O}$. In the above quantity, the summand with $(V^{(12)})_{11}$ can be estimated with the very same arguments used for the control of the first summand in the r.h.s. of (4.60) above, that is,

$$\begin{aligned}\big|\big\langle\psi, q_1^A p_1^B (V^{(12)})_{11} q_1^A q_1^B p_2^A\,\psi\big\rangle\big| \;&\leqslant\; \|(V^{(12)})_{11} q_1^A p_1^B \psi\|\,\|q_1^A q_1^B p_2^A\psi\| \\ &\leqslant\; \sqrt{\langle\psi, q_1^A p_1^B (V_{12}^2)_{11} q_1^A p_1^B\,\psi\rangle}\,\sqrt{\langle\psi, q_1^A q_1^B\,\psi\rangle} \\ &\leqslant\; \sqrt{\langle\psi, q_1^A p_1^B (V_{12}^2 * |v|^2)_1^A q_1^A p_1^B\,\psi\rangle}\,\sqrt{\|q_1^A\psi\|\,\|q_1^B\psi\|} \\ &\leqslant\; \sqrt{\|V_{12}^2 * |v|^2\|_\infty}\;\alpha^{(1,1)} \\ &\leqslant\; \sqrt{2}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|v\|_{\widehat{r}_{12}} + \|v\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\,.\end{aligned}$$

The summand with $(V^{(12),u})_1^B$ is estimated via a Cauchy-Schwarz inequality and the bound (4.27) of Lemma 4.8 as

$$\begin{aligned}|\langle\psi, q_1^A p_1^B\,(V^{(12),u})_1^B\, q_1^A q_1^B p_2^A\,\psi\rangle| \;&\leqslant\; \|V^{(12)} * |u|^2\|_\infty\,\|q_1^A\psi\|\,\|q_1^B\psi\| \\ &\leqslant\; \sqrt{2}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}} + \|u\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\,.\end{aligned}$$

Therefore, since $(N_1-1)(N)^{-1} \leqslant c_1 \leqslant 1$,

$$|(qp,qq)| \;\lesssim\; \|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}} + \|u\|_{\widehat{s}_{12}} + \|v\|_{\widehat{r}_{12}} + \|v\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\,.$$

The very same discussion above for (qp,qq) can be repeated for the term (pq,qq) in (4.56). Thus,

$$\begin{aligned}|(qp,qq)| + |(pq,qq)| \;&\lesssim\; \|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\times \\ &\qquad\times\big(\|u\|_{\widehat{r}_{12}} + \|u\|_{\widehat{s}_{12}} + \|v\|_{\widehat{r}_{12}} + \|v\|_{\widehat{s}_{12}}\big)\,\alpha^{(1,1)}\,.\end{aligned}\tag{4.62}$$

It remains to control the term (pp,qq) in (4.56). One has

$$\begin{aligned}&\frac{N_1 N_2}{N}\,\Big\langle\psi, p_1^A p_1^B\Big[(V^{(12)})_{11} - (V^{(12),v})_1^A - (V^{(12),u})_1^B\,,\,\sum_{k=1}^{N_1}\sum_{\ell=1}^{N_2}\frac{p_k^A\,p_\ell^B}{N_1N_2}\Big]q_1^A q_1^B\psi\Big\rangle \\ &=\;\frac{1}{N}\,\Big\langle\psi, p_1^A p_1^B\Big[(V^{(12)})_{11}\,,\,\sum_{k=1}^{N_1} p_k^A\,p_1^B + \sum_{\ell=1}^{N_2} p_1^A\,p_\ell^B - p_1^A p_1^B\Big]q_1^A q_1^B\psi\Big\rangle \\ &=\;\frac{N_1-1}{N}\,\langle\psi, p_1^A p_1^B\big[(V^{(12)})_{11}\,,\,p_2^A p_1^B\,\big]q_1^A q_1^B\psi\rangle \\ &\qquad+\frac{N_2-1}{N}\,\langle\psi, p_1^A p_1^B\big[(V^{(12)})_{11}\,,\,p_1^A p_2^B\,\big]q_1^A q_1^B\psi\rangle \\ &\qquad+\frac{1}{N}\,\langle\psi, p_1^A p_1^B\big[(V^{(12)})_{11}\,,\,p_1^A p_1^B\,\big]q_1^A q_1^B\psi\rangle \\ &\equiv\;(pp,qq)_1 + (pp,qq)_2 + (pp,qq)_3\,,\end{aligned}$$

where in the first identity we applied (4.59) and we dropped the $(V^{(12),v})_1^A$-term (respectively, the $(V^{(12),u})_1^B$-term) owing to the commutation of q_1^B (resp., q_1^A) from the right all the way through to the left with $p_1 q_1 = \mathbb{O}$, and in the second identity we used the symmetry of ψ.

One has

$$\begin{aligned}
(pp,qq)_1 &= \frac{N_1-1}{N}\,\langle\psi, p_1^A p_1^B\big[(V^{(12)})_{11}\,,\,p_2^A p_1^B\,\big]q_1^A q_1^B\psi\rangle \\
&= -\frac{N_1-1}{N}\,\langle\psi, p_1^A p_1^B\,(V^{(12)})_{11}\,p_2^A q_1^A q_1^B\psi\rangle \\
&= -\frac{N_1-1}{N}\,\langle\psi, p_1^A p_1^B\,(V^{(12)})_{11}\,\widehat{n}^A(\widehat{n}^{-1})^A p_2^A q_1^A q_1^B\psi\rangle \\
&= -\frac{N_1-1}{N}\,\langle\psi, p_1^A p_1^B\,\widehat{\tau_1 n}^A(V^{(12)})_{11}(\widehat{n}^{-1})^A p_2^A q_1^A q_1^B\psi\rangle
\end{aligned}$$

where in the third step we introduced the auxiliary operator $\widehat{n}$ defined in (4.69) and (4.71), using again the fact that $(\widehat{n}^{-1})^A$ is well defined on the range of q_1^A, and in the last step we applied Lemma 4.13 in the form (4.81). Therefore,

$$\begin{aligned}
|(pp,qq)_1| &\leqslant |\langle\psi, p_1^A p_1^B\,\widehat{\tau_1 n}^A(V^{(12)})_{11}(\widehat{n}^{-1})^A p_2^A q_1^A q_1^B\,\psi\rangle| \\
&\leqslant \sqrt{\langle\psi, p_1^A p_1^B\,\widehat{\tau_1 n}^A(V_{12}^2)_{11}\,\widehat{\tau_1 n}^A p_1^A p_1^B\,\psi\rangle}\,\sqrt{\langle\psi,(\widehat{n}^{-2})^A p_2^A q_1^A q_1^B\,\psi\rangle} \\
&\leqslant 2\sqrt{\langle\psi, p_1^A p_1^B\,\widehat{\tau_1 n}^A(V_{12}^2*|v|^2)_1^B\,\widehat{\tau_1 n}^A p_1^A p_1^B\,\psi\rangle}\,\|q_1^B\,\psi\| \\
&\leqslant 2\sqrt{\|V_{12}^2*|v|^2\|_\infty}\,\sqrt{\langle\psi,\widehat{\tau_1 m}^A\psi\rangle}\,\sqrt{\alpha^{(1,1)}} \\
&= 2\sqrt{\|V_{12}^2*|v|^2\|_\infty}\,\sqrt{\Big\langle\psi,\Big(\widehat{m}^A+\frac{1}{N_1}\Big)\psi\Big\rangle}\,\sqrt{\alpha^{(1,1)}} \\
&= 2\sqrt{\|V_{12}^2*|v|^2\|_\infty}\,\sqrt{\alpha^{(1,1)}+\frac{1}{N_1}}\,\sqrt{\alpha^{(1,1)}} \\
&\leqslant \frac{4\sqrt{2}}{c_1}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)
\end{aligned}$$

where in the first step we used the bound $(N_1-1)(N)^{-1}\leqslant c_1\leqslant 1$, in the second we applied the Cauchy-Schwarz inequality, in the third we used (4.25) and (4.71), as well as Lemma 4.12 in the form (4.78), in the fourth we used again (4.71) and $\|q_1^A\psi\|^2=\alpha^{(1,0)}\leqslant\alpha^{(1,1)}$ ((1.9) of Lemma 1.1), in the fifth we used (4.69), in the sixth we used (4.72) and again $\|q_1^A\psi\|^2\leqslant\alpha^{(1,1)}$, and in the last we applied (4.27) of Lemma 4.8 and

$$\begin{aligned}
\sqrt{\alpha^{(1,1)}+\frac{1}{N_1}}\,\sqrt{\alpha^{(1,1)}} &\leqslant \alpha^{(1,1)}+\frac{1}{2N_1} \leqslant \frac{N}{N_1}\Big(\alpha^{(1,1)}+\frac{1}{N}\Big) \\
&\leqslant \frac{2}{c_1}\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)\,.
\end{aligned}$$

With the very same arguments one finds

$$|(pp,qq)_2| \leqslant \frac{2\sqrt{2}}{c_2}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}\big)\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)\,.$$

Last,

$$\begin{aligned}
|(pp,qq)_3| &= \Big|\frac{1}{N}\Big\langle\psi, p_1^A p_1^B\,\big[(V^{(12)})_{11}\,,\,p_1^A p_1^B\,\big]\,q_1^A q_1^B\psi\Big\rangle\Big| \\
&\leqslant \frac{1}{N}\,|\langle\psi, p_1^A p_1^B\,(V^{(12)})_{11}\,q_1^A q_1^B\psi\rangle| \\
&\leqslant \frac{1}{N}\sqrt{\langle\psi, p_1^A p_1^B\,(V_{12}^2)_{11}\,p_1^A p_1^B\psi\rangle} \\
&= \frac{1}{N}\sqrt{\langle\psi, p_1^A p_1^B\,(V_{12}^2*|u|^2)_1^A\,p_1^A p_1^B\psi\rangle} \\
&\leqslant \frac{1}{N}\sqrt{\|V_{12}^2*|u|^2\|_\infty} \\
&\leqslant \frac{\sqrt{2}}{N}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}\big)
\end{aligned}$$

where the second step follows by $pq=\mathbb{O}$, the third by a Cauchy-Schwarz inequality and the operator bound $\mathbb{O}\leqslant q\leqslant\mathbb{1}$, the fourth by (4.25), the fifth by $\mathbb{O}\leqslant p\leqslant\mathbb{1}$, and the last by (4.27).

Therefore,

$$\begin{aligned}
|(pp,qq)| &\leqslant |(pp,qq)_1|+|(pp,qq)_2|+|(pp,qq)_3| \\
&\leqslant \widetilde{\kappa}_{12}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}+\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\times \\
&\qquad\times\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)
\end{aligned}\tag{4.63}$$

where the constant $\widetilde{\kappa}_{12}$ only depends on the population fractions c_1 and c_2.

Plugging (4.62) and (4.63) into (4.56), which are the only non-zero contributions to Ω, and renaming $\widetilde{\kappa}_{12}$, we finally obtain

$$\begin{aligned}
|\Omega| &\leqslant \widetilde{\kappa}_{12}\,\|V^{(12)}\|_{L^{r_{12}}+L^{s_{12}}}\big(\|u\|_{\widehat{r}_{12}}+\|u\|_{\widehat{s}_{12}}+\|v\|_{\widehat{r}_{12}}+\|v\|_{\widehat{s}_{12}}\big)\times \\
&\qquad\times\Big(\alpha^{(1,1)}+\frac{1}{N}\Big)\,.
\end{aligned}\tag{4.64}$$

4.4 Tools exported from the single-component treatment

We collect here a number of definitions and useful results needed in the proof of Theorem 4.1, on which the "counting" method is based, quoting their properties from the previous treatments of the single-component case [44], [83], [81], [82].

Consider the projections

$$p\;:=\;|\phi\rangle\langle\phi|\,,\qquad q\;:=\;\mathbb{1}-|\phi\rangle\langle\phi|\tag{4.65}$$

on a one-body Hilbert space $\mathfrak{h}$ and their realization p_j, q_j, $j\in\{1,\dots,N\}$ as orthogonal projections on the many-body Hilbert space $\mathcal{H}_N=\mathfrak{h}^{\otimes N}$, where $\phi\in\mathfrak{h}$ with $\|\phi\|=1$. Clearly, $p+q=\mathbb{1}$ and $pq=\mathbb{O}=[p,q]$.

Associated to p and q one defines the family of orthogonal projections P_k acting on $\mathcal{H}_N$, defined by

$$\begin{aligned}
P_k &:= \sum_{\substack{a\in\{0,1\}^N\\ \sum_i a_i=k}}\;\prod_{i=1}^N p_i^{1-a_i}q_i^{a_i} \qquad \text{if } k\in\{0,1,\dots,N\} \\
P_k &:= \mathbb{O} \qquad\qquad\qquad\qquad\quad \text{otherwise}\,.
\end{aligned}\tag{4.66}$$

Each P_k consists by construction of the sum of all possible N-fold tensor products of the p's and the q's with k factor q. It therefore arises as the k-th term in the expansion of the identity

$$\mathbb{1} \;=\; (p_1+q_1)\cdots(p_N+q_N) \;=\; \sum_{k=0}^{N} P_k \tag{4.67}$$

in powers of q. It is also clear by the commutation properties of the p_j's and q_j's that

$$P_k\,P_\ell \;=\; \delta_{k,\ell}P_k\,. \tag{4.68}$$

A relevant role is played by suitable weighted linear combinations of the P_k's. To this aim one introduces, associated to any function $f:\{0,1,\dots,N\}\to\mathbb{C}$, i.e., any $(N+1)$-ple $(f(0),\dots,f(N))\in\mathbb{C}^{N+1}$, the operator

$$\widehat{f} \;:=\; \sum_{k=0}^{N} f(k)\,P_k\,. \tag{4.69}$$

As an immediate consequence of (4.68) and of the commutation properties of the p_j's,

$$[\,\widehat{f}\,,\,p_j\,] \;=\; [\,\widehat{f}\,,\,P_k\,] \;=\; \mathbb{O}\,,\qquad [\,\widehat{f}\,,\,\widehat{g}\,] \;=\; \mathbb{O}\,. \tag{4.70}$$

Two convenient choices for the function f shall be

$$m(k) \;:=\; \frac{k}{N}\,,\qquad n(k) \;:=\; \sqrt{\frac{k}{N}}\,. \tag{4.71}$$

For the operator $\widehat{m}$ one has

$$\frac{1}{N}\sum_{j=1}^{N} q_j \;=\; \frac{1}{N}\sum_{k=0}^{N}\sum_{j=1}^{N} q_jP_k \;=\; \frac{1}{N}\sum_{k=0}^{N} kP_k \;=\; \widehat{m}\,. \tag{4.72}$$

Therefore, if $\psi\in\mathcal{H}_{N,\mathrm{sym}}\equiv(\mathfrak{h}^{\otimes N})_{\mathrm{sym}}$, then (4.72) implies

$$\langle\psi,q_1\,\psi\rangle \;=\; \langle\psi,\widehat{m}\,\psi\rangle\,. \tag{4.73}$$

We thus come to the following useful bounds (see [44, Lemma 3.9]):

Lemma 4.11. *For any $f:\{0,\dots,N\}\to[0,+\infty)$ and any $\psi\in\mathcal{H}_{N,\mathrm{sym}}$ one has*

$$\langle\psi,\widehat{f}\,q_1\,\psi\rangle \quad = \quad \langle\psi,\widehat{f}\,\widehat{m}\,\psi\rangle \tag{4.74}$$

$$\langle\psi,\widehat{f}\,q_1\,q_2\,\psi\rangle \quad \leqslant \quad \frac{N}{N-1}\langle\psi,\widehat{f}\,\widehat{m}^2\,\psi\rangle\,. \tag{4.75}$$

A further relevant tool is a modification of Lemma 4.11 above for the case when ψ carries only a partial permutation symmetry. In the present context this is the case when we consider the two-component many-body states of the form $p_1^A\psi$ – see the control of terms of the form $(pp,qq)_1$ in Subsection 4.3.3. We import the following result from [82, Lemma 4.2]:

Lemma 4.12. *For any $f:\{0,\dots,N\}\to[0,+\infty)$ and any $\Phi\in\mathfrak{h}\otimes\mathcal{H}_{N-1,\mathrm{sym}}$ one has*

$$\|\widehat{f}q_1\Phi\|^2 \;\leqslant\; \frac{N}{N-1}\,\|\widehat{f}\,\widehat{n}\,\Phi\|^2\,. \tag{4.76}$$

In particular, in the context of Subsection 4.3.2, the bound (4.76) above implies

$$\begin{aligned}\langle\psi,(\widehat{n}^{-2})^A q_1^A q_2^A p_1^B \psi\rangle &\leqslant \|(\widehat{n}^{-1})^A q_1^A q_2^A p_1^B\,\psi\|^2 \\ &\leqslant \frac{N_1}{N_1-1}\,\|(\widehat{n}^{-1})^A\,\widehat{n}^A q_2^A p_1^B\,\psi\|^2 \\ &\leqslant 2\,\|q_2^A\psi\|^2\end{aligned}\tag{4.77}$$

and similarly, in the context of Subsection 4.3.3,

$$\begin{aligned}\langle\psi,(\widehat{n}^{-2})^A p_2^A q_1^A q_1^B\,\psi\rangle &= \|(\widehat{n}^{-1})^A q_1^A q_1^B p_2^A\,\psi\|^2 \\ &\leqslant \frac{N_1}{N_1-1}\,\|(\widehat{n}^{-1})^A\,\widehat{n}^A p_2^A q_1^B\,\psi\|^2 \\ &\leqslant 2\,\|q_1^B\psi\|^2\,.\end{aligned}\tag{4.78}$$

Next to the operators of the form $\widehat{f}$, a relevant role in the estimates for the "counting" method is played by the operators of the form $\widehat{\tau_n f}$, where τ_n for given $n\in\mathbb{Z}$ is the operation that produces the shifted function

$$(\tau_n f)(k) \;:=\; f(k+n)\,,\qquad k\in\{0,1,\dots,N\}\,.\tag{4.79}$$

The following important property holds (see [44, Lemma 3.10]):

Lemma 4.13. *Let $A_{1\cdots r}\equiv A\otimes\mathbb{1}_{N-r}$ be an operator on $\mathcal{H}_N\cong\mathcal{H}_r\otimes\mathcal{H}_{N-r}$ that acts non-trivially only on the first factor $\mathcal{H}_r$, and let Q_j, $j=1,2$, be two orthogonal projections on $\mathcal{H}_r$ given by monomials of p's and q's, each with n_j factors q and $r-n_j$ factors p. Set $n:=n_2-n_1$. Then*

$$Q_1\,A_{1\dots r}\,\widehat{f}\,Q_2 \;=\; Q_1\,\widehat{\tau_n f}\,A_{1\dots r}\,Q_2\tag{4.80}$$

as an identity of bounded operators on $\mathcal{H}_N$ (with a tacit identification $Q_j\equiv Q_j\otimes\mathbb{1}_{N-r}$).

In fact, as a consequence of the presence of only *two-body* interactions in the many-body Hamiltonian H_N^{MF}, the use of Lemma 4.13 is in practice limited to the case $r=2$: formula (4.80) then reads

$$\begin{aligned}p_1\,p_2\,A_{12}\,\widehat{f}\,q_1\,p_2 &= p_1\,p_2\,\widehat{\tau_1 f}\,A_{12}\,q_1\,p_2 \\ p_1\,p_2\,A_{12}\,\widehat{f}\,q_1\,q_2 &= p_1\,p_2\,\widehat{\tau_2 f}\,A_{12}\,q_1\,q_2 \\ q_1\,p_2\,A_{12}\,\widehat{f}\,q_1\,q_2 &= q_1\,p_2\,\widehat{\tau_1 f}\,A_{12}\,q_1\,q_2\end{aligned}\tag{4.81}$$

while in all other cases with equal number of q's on the left and on the right we have a commutation of the form $\sharp_1\sharp_2 A_{12}\,\widehat{f}\,\sharp_1\sharp_2=\sharp_1\sharp_2\,\widehat{f}\,A_{12}\,\sharp_1\sharp_2$.

Chapter 5

Further topics

In this Chapter we present some further topics concerning the study and derivation of effective theories for many-body systems. The results presented are based on my papers [66], [65], both in collaboration with Michelangeli, [68], with Michelangeli and Scandone, and [78]. Even though they constitute an important part of my work, they cannot be extensively discussed in the space of the present thesis. Hence, they are surveyed in this Chapter, with introductions, main statements, and discussions, but no proofs.

5.1 Effective dynamics for (pseudo-)spinor condensates

This Section is based on my works [66], [65].

Gases of ultra-cold bosons which macroscopically occupy a single one-body state and have internal spin degrees of freedom are often called *(pseudo-)spinor condensates* . The term pseudo-spinor is adopted when particles are not coupled by a genuine spin-spin interaction, while still coupled to an external micro-wave or radio-frequency radiation field. When, in turn, particles undergo an additional spin-spin interaction, the term *spinor condensate* is adopted. In both cases, the condensate wave-function is a multi-component spinor, and the dynamical evolution observed in the experiments shows an excellent matching with a system of non-linear coupled equations for the condensate wave-function.

We refer to [72], [62], [37], [38] for experimental realizations of condensates with different hyperfine states of ^{87}Rb, and to the reviews [90], [60], [36], [91], [84] for an outlook on the huge amount of experimental and theoretical studies.

We will consider systems of N identical spin-m bosons in three dimensions, whose Hilbert space is

$$\mathcal{H}_N^{(m)} \;:=\; \big(L^2(\mathbb{R}^3)\otimes\mathbb{C}^{2m+1}\big)^{\otimes_{\mathrm{sym}}N}\,. \tag{5.1}$$

We shall specialize this to $m=2$ for the case of pseudo-spinor condensates and to $m=3$ for spinor condensates, because, respectively, 2 and 3 hyperfine levels are effectively relevant to the phenomena we describe. Hence

$$\mathcal{H}_N^{\mathrm{ps}} \;:=\; \mathcal{H}_N^{(2)}, \qquad \mathcal{H}_N^{\mathrm{s}} \;:=\; \mathcal{H}_N^{(3)}. \tag{5.2}$$

We will first present our result on the derivation of the effective dynamics of pseudo-spinor condensates in the Gross-Pitaevskii regime and with time-dependent magnetic fields, which we proved in the work [66]. After this, we will state the corresponding result for spinor condensates in the mean-field regime, based on our work [65]. A further result on the effective dynamics of spinor condensates in the GP regime is contained in our work [65], but we shall not report it here.

We let the system of pseudo-spinors be governed by the Hamiltonian

$$H_N^{\mathrm{ps}} \;=\; \sum_{j=1}^{N}(-\Delta_{x_j}+S(x_j,t))+N^2\sum_{j<k}^{N}V(N(x_j-x_k)), \tag{5.3}$$

acting self-adjointly on $\mathcal{H}_N^{\mathrm{ps}}$, where the operator S on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ is defined by

$$S(x,t) \;:=\; \begin{pmatrix} U_\uparrow^{\mathrm{trap}}(x)-V_{\mathrm{hf}}(x,t) & B_1(x,t)-\mathrm{i}B_2(x,t) \\ & \\ B_1(x,t)+\mathrm{i}B_2(x,t) & U_\downarrow^{\mathrm{trap}}(x)+V_{\mathrm{hf}}(x,t) \end{pmatrix}. \tag{5.4}$$

H_N^{ps} consists of the sum of N one-body Hamiltonians containing a kinetic part, an external spatial trapping potential, and an interaction between the spin of each particle and an external magnetic field $\mathbf{B}=(B_1,B_2,-V_{\mathrm{hf}})$, plus a potential part, made of two-body pair interactions in the Gross-Pitaevskii regime. Notice that the notation V_{hf} referring to a field causing a splitting between the $h$yper$f$ine levels is consistent with experimental literature.

Let us consider the Cauchy problem for the associated (linear) Schrödinger equation

$$\begin{cases} \mathrm{i}\partial_t\psi_{N,t} &= H_N^{\mathrm{ps}}\psi_{N,t} \\ \psi_{N,t}|_{t=0} &= \psi_N \end{cases} \tag{5.5}$$

for a given initial datum ψ_N. Since H_N^{ps} may depend on time, suitable conditions on $S(x,t)$ will be assumed so as to ensure that the solution to (5.5) exists and is unique in the strong sense for any time.

To investigate the effective dynamics generated by H_N^{ps} we are concerned with initial data exhibiting condensation onto some condensate spinor (see Assumption (A_5^{ps})). Moreover, since we are considering the Gross-Pitaevskii regime, the initial datum needs be energetically compatible with the effective theory (see again Assumption (A_5^{ps})). This requirement, which selects ground state-like states (and hence preparable states) as initial data, is expressed in terms of the many-body energy per particle

$$\mathcal{E}_N^{\mathrm{ps}}[\psi_N] \;:=\; \frac{1}{N}\langle\psi_N, H_N^{\mathrm{ps}}\psi_N\rangle\,, \qquad \psi_N\in\mathcal{H}_N^{\mathrm{ps}}\,, \tag{5.6}$$

and of the Gross-Pitaevskii energy functional

$$\begin{aligned}\mathcal{E}^{\mathrm{GP,ps}}[u,v] \;:=\; &\int_{\mathbb{R}^3}\Big(|\nabla u|^2+|\nabla v|^2+4\pi a\big(|u|^4+2|u|^2|v|^2+|v|^4\big)\Big)\,\mathrm{d}x \\ &+\Big\langle\begin{pmatrix}u\\v\end{pmatrix},\,S(t)\begin{pmatrix}u\\v\end{pmatrix}\Big\rangle_{L^2(\mathbb{R}^3)\otimes\mathbb{C}^2} \qquad u,v\in L^2(\mathbb{R}^3)\,,\end{aligned} \tag{5.7}$$

where a is the (s-wave) scattering length associated to the potential V.

Our result will state that condensation is preserved along the dynamics ruled by (5.5), and, for $t>0$, the effective dynamics for the spinor wave-function of the condensate is ruled by the system of non-linear Schrödinger equations [90], [60], [36], [91], [84]

$$\begin{cases} i\partial_t u_t &= h_{11}^{(u,v)}u_t+S_{12}v_t \\ i\partial_t v_t &= h_{22}^{(u,v)}v_t+S_{21}u_t\,, \end{cases} \tag{5.8}$$

having introduced the 'one-body non-linear Hamiltonians'

$$\begin{aligned} h_{11}^{(u,v)} &:= -\Delta + U_{\uparrow}^{\mathrm{trap}} + 8\pi a(|u_t|^2+|v_t|^2) - V_{\mathrm{hf}} \;=\; -\Delta + S_{11} + 8\pi a(|u_t|^2+|v_t|^2) \\ h_{22}^{(u,v)} &:= -\Delta + U_{\downarrow}^{\mathrm{trap}} + 8\pi a(|u_t|^2+|v_t|^2) + V_{\mathrm{hf}} \;=\; -\Delta + S_{22} + 8\pi a(|u_t|^2+|v_t|^2). \end{aligned} \tag{5.9}$$

We impose the following set of assumptions:

(A_1^{ps}) The matrix potential $S \equiv (S_{jk})_{j,k\in\{1,2\}}$ be given with $S_{ij} \in W^{1,\infty}(\mathbb{R}_t, L^\infty_x(\mathbb{R}^3))$ and $S = S^*$.

(A_2^{ps}) The real-valued unscaled potential V be given such that $V \in L^\infty(\mathbb{R}^3)$ with compact support, and for almost every $x \in \mathbb{R}^3$, V is spherically symmetric and non-negative.

(A_3^{ps}) Associated to the potentials fixed in (A_1^{ps})-(A_2^{ps}), let H_N^{ps} be the many-body Hamiltonian (5.3) acting at each time t on the N-body Hilbert space $\mathcal{H}_N^{\mathrm{ps}}$ fixed in (5.1), let $\mathcal{E}_N$ be the the many-body energy-per-particle functional (5.6), and let $\mathcal{E}^{\mathrm{GP,ps}}$ be the two-component Gross-Pitaevskii energy functional (5.7).

(A_4^{ps}) Two functions $u, v \in H^2(\mathbb{R}^3)$ be given with $\|u\|^2 + \|v\|^2 = 1$ and such that the Cauchy problem associated to the non-linear system (5.8) with initial datum (u, v) admits a unique solution (u_t, v_t)

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} \in C\big(\mathbb{R}_t, H^2_x(\mathbb{R}^3) \otimes \mathbb{C}^2\big)\,. \tag{5.10}$$

(A_5^{ps}) Associated to the spinor $\begin{pmatrix} u \\ v \end{pmatrix}$ fixed in (A_4^{ps}), an initial N-body $\psi_N \in \mathcal{H}_N^{\mathrm{ps}}$ be given, with $\|\psi_N\| = 1$, such that

$$\mathrm{Tr}\left|\gamma_{\psi_N}^{(1)} - \left|\begin{pmatrix} u \\ v \end{pmatrix}\right\rangle\!\left\langle\begin{pmatrix} u \\ v \end{pmatrix}\right|\right| \;\leqslant\; \frac{\mathrm{const.}}{N^{\eta_1}} \tag{5.11}$$

and

$$\big|\, \mathcal{E}_N^{\mathrm{ps}}[\psi_N] \to \mathcal{E}^{\mathrm{GP,ps}}[u,v]\,\big| \;\leqslant\; \frac{\mathrm{const.}}{N^{\eta_2}} \tag{5.12}$$

for some constants $\eta_1, \eta_2 > 0$. Here $\gamma_{\psi_N}^{(1)}$ is obtained by tracing out, from the state γ_{ψ_N}, the space and spin degrees of freedom of all particles but one.

Some remarks are in order. First (A_5^{ps}) is expected to select the class of initial states relevant in the experiments, i.e., initially prepared condensates whose energy is compatible with the effective Gross-Pitaevskii description. Moreover, we underline that assumption (A_1^{ps}) includes the experimentally interesting potentials $V_{\mathrm{hf}}(x) \equiv V_{\mathrm{hf}}$ and $S_{12}(x,t) = B_1(x,t) - \mathrm{i}B_2(x,t) \equiv \Omega e^{\mathrm{i}\omega t}$ for suitable constants $V_{\mathrm{hf}}, \Omega, \omega \geqslant 0$.

As a further important remark, we observe that both dynamical evolutions we deal with in our assumptions, namely the linear many-body Schrödinger dynamics and the non-linear Gross-Pitaevskii dynamics, are well posed. Concerning the former, it can be deduced from (A_3^{ps}) by means of standard arguments (see, e.g., [1] for a recent discussion) that H_N^{ps} has a time-independent (dense) domain $\mathcal{D}_N \subset \mathcal{H}_N^{\mathrm{ps}}$ of self-adjointness and there exists a unique unitary propagator for (5.5) on $\mathcal{H}_N^{\mathrm{ps}}$, that is, a family $\{U_N(t,s)\,|\,t,s\in\mathbb{R}\}$ of unitaries on $\mathcal{H}_N^{\mathrm{ps}}$, strongly continuous with respect to (t,s), satisfying $U_N(t,s)U_N(s,r) = U_N(t,r)$ and $U_N(t,t) = \mathbb{1}$ for any $t,s,r \in \mathbb{R}$, and with the additional properties that, equipping $\mathcal{D}_N$ with the graph norm of $H_N^{\mathrm{ps}}|_{t=0}$, each $U_N(t,s)$ is bounded on $\mathcal{D}$, and for each $\Phi_N \in \mathcal{D}_N$ the function $U_N(t,s)\Phi_N$ is continuous in $\mathcal{D}_N$ with respect to (t,s), it is of class C^1 in $\mathcal{H}_N$, and

$$\mathrm{i}\partial_t U_N(t,s)\Phi_N \;=\; H_N^{\mathrm{ps}} U_N(t,s)\Phi_N\,, \qquad \mathrm{i}\partial_s U_N(t,s)\Phi_N \;=\; -U_N(t,s)H_N^{\mathrm{ps}}\Phi_N\,. \tag{5.13}$$

The non-linear Cauchy problem associated to (5.8) is well-posed too (in fact, it is defocusing and energy sub-critical), which is seen by exploiting an amount of standard analysis that can be found in the closely related works [43], [7], [16]. It has to be stressed that we do make the for us technically crucial assumption that the solution (u,v) has H^2-norm uniformly bounded in time.

We are now in the condition to state our main result of persistence in time of pseudo-spinorial BEC and rigorous derivation of the non-linear effective dynamics. It is formulated as follows.

Theorem 5.1. *Consider a system consisting of N spin-$\frac{1}{2}$ identical bosons in three dimensions, subject to the Hamiltonian H_N^{ps} and initialized at time $t=0$ in the state ψ_N of complete BEC onto the one-body spinor $\begin{pmatrix} u \\ v \end{pmatrix}$, according to the assumptions (A_1^{ps})-(A_5^{ps}) above. For each $t>0$ let $\psi_{N,t}$ be the solution to the many-body Schrödinger equation* (5.5) *with initial datum ψ_N, let $\gamma^{(1)}_{\psi_{N,t}}$ be the associated one-body reduced density matrix, and let (u_t,v_t) be the solution to the non-linear Gross-Pitaevskii system* (5.8) *with initial datum (u,v). Then, at any t,*

$$\lim_{N\to\infty}\gamma^{(1)}_{\psi_{N,t}} \;=\; \Big|\begin{pmatrix} u_t \\ v_t \end{pmatrix}\Big\rangle\Big\langle\begin{pmatrix} u_t \\ v_t \end{pmatrix}\Big| \tag{5.14}$$

in trace norm, and

$$\lim_{N\to\infty}\mathcal{E}_N^{\mathrm{ps}}[\psi_{N,t}] \;=\; \mathcal{E}^{\mathrm{GP,ps}}[u_t,v_t]\,. \tag{5.15}$$

It is worth remarking that the convergence in (5.14) and (5.15) hold with a rate $N^{-\eta}$, with $\eta>0$ depending on η_1,η_2 of (A_5^{ps}). Such rate is however certainly non-optimal, and hence we omit to keep track of it.

The proof of Theorem 5.1 can be found in [66]. It goes through a suitable adaptation of the counting projection method developed by Pickl [44], [83], [81], [82].

Let us now discuss the case of *spinor condensates*, where now a spin-spin coupling is present. We set-up the model in the concrete case of spin-1 bosons (see [19] for a modern experimental realization) and present the result of derivation of the effective dynamics in the mean-field regime.

The many-body Hilbert space for spin-1 bosons is, as already anticipated,

$$\mathcal{H}_N^{\mathrm{s}} \;:=\; \big(L^2(\mathbb{R}^3)\otimes\mathbb{C}^3\big)^{\otimes_{\mathrm{sym}}N}, \tag{5.16}$$

on which acts the mean-field many-body Hamiltonian

$$\begin{aligned} H_N^{\mathrm{s}} \;:=\; & \sum_{j=1}^N(-\Delta_{x_j}) + \frac{1}{N}\sum_{1<j\leqslant k<N} W(x_j-x_k) \\ & + \frac{1}{N}\sum_{1<j\leqslant k<N} V(x_j-x_k)\,\boldsymbol{\sigma}_j\bullet\boldsymbol{\sigma}_k. \end{aligned} \tag{5.17}$$

Here we are denoting collectively by $\boldsymbol{\sigma}$ the symbolic vector $\boldsymbol{\sigma}=(\sigma^{(1)},\sigma^{(2)},\sigma^{(3)})$, where

$$\sigma^{(1)} \;=\; \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \sigma^{(2)} \;=\; \frac{-\mathrm{i}}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad \sigma^{(3)} \;=\; \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

are the usual Pauli matrices on $\mathbb{C}^3$. With respect to the tensor product $(\mathbb{C}^3)^{\otimes N}$ the notation $\boldsymbol{\sigma}_j = (\sigma_j^{(1)}, \sigma_j^{(2)}, \sigma_j^{(3)})$ is going to be used to indicate the operator that acts as $\boldsymbol{\sigma}$ on the j-th copy of the tensor product (the j-th spin degree of freedom), and trivially as the identity on all other copies. Analogously the notation $\boldsymbol{\sigma}_j \bullet \boldsymbol{\sigma}_k$, for given $j,k \in \{1,\dots,N\}$, is a short-cut for the operator

$$\boldsymbol{\sigma}_j \bullet \boldsymbol{\sigma}_k \;=\; \sigma_j^{(1)} \otimes \sigma_k^{(1)} + \sigma_j^{(2)} \otimes \sigma_k^{(2)} + \sigma_j^{(3)} \otimes \sigma_k^{(3)}\,,$$

understanding $A_j \otimes B_k$ as an operator acting non-trivially only on the j-th and the k-th copy of the tensor product space.

We refer to [76], [40], [45], [65] for discussions on the validity of the model and on the physical role of the potentials V and W, as well as for theoretical investigation on the properties of H_N^{s}.

Let us consider the Cauchy problem for the (linear) Schrödinger equation

$$\begin{cases} \mathrm{i}\partial_t \psi_{N,t} \;=\; H_N^{\mathrm{s}} \psi_{N,t} \\ \psi_{N,t}|_{t=0} \;=\; \psi_N \end{cases} \tag{5.18}$$

for a given initial datum $\psi_N \in \mathcal{H}_N^{\mathrm{s}}$ that exhibits complete BEC, i.e. such that there exist $u,v,w \in L^2(\mathbb{R}^3)$ such that

$$\begin{aligned} \lim_{N\to\infty} \gamma_{\psi_N}^{(1)} \;&=\; \left| \begin{pmatrix} u \\ v \\ w \end{pmatrix} \right\rangle \left\langle \begin{pmatrix} u \\ v \\ w \end{pmatrix} \right|\,, \qquad \phi = \begin{pmatrix} u \\ v \\ w \end{pmatrix}\,, \\ \|\phi\|_{\mathfrak{h}} \;&=\; \|u\|^2_{L^2(\mathbb{R}^3)} + \|v\|^2_{L^2(\mathbb{R}^3)} + \|w\|^2_{L^2(\mathbb{R}^3)} \;=\; 1. \end{aligned} \tag{5.19}$$

It is an extensive experimental evidence that under suitable conditions, and with very good approximation, spinor BEC persists at later times onto some spinor ϕ_t whose components solve the mean-field non-linear Schrödinger spinor system, or *spinor Hartree system* for short,

$$\begin{aligned} \mathrm{i}\partial_t u_t \;&=\; -\Delta u_t + (W * (|u_t|^2 + |v_t|^2 + |w_t|^2))u_t \\ &\quad + (V * |u_t|^2)u_t - (V * |w_t^2|)u_t + (V * (\overline{v_t} u_t))v_t + (V * (\overline{w_t} v_t))v_t \\ \mathrm{i}\partial_t v_t \;&=\; -\Delta u_t + (W * (|u_t|^2 + |v_t|^2 + |w_t|^2))v_t \\ &\quad + (V * (\overline{u_t} v_t))u_t + (V * (\overline{v_t} w_t))u_t + (V * (\overline{v_t} u_t))w_t + (V * (\overline{w_t} v_t))w_t \\ \mathrm{i}\partial_t w_t \;&=\; -\Delta u_t + (W * (|u_t|^2 + |v_t|^2 + |w_t|^2))w_t \\ &\quad + (V * |w_t|^2)w_t - (V * |u_t^2|)w_t + (V * (\overline{u_t} v_t))v_t + (V * (\overline{v_t} w_t))v_t. \end{aligned} \tag{5.20}$$

It is not difficult to infer that the system is well-posed in $H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3) \oplus H^1(\mathbb{R}^3)$ if, for instance, $V^2 \lesssim (\mathbb{1} - \Delta)$ and $W^2 \lesssim (\mathbb{1} - \Delta)$ in the sense of forms of operators on $L^2(\mathbb{R}^3)$.

Our main result takes the following form.

Theorem 5.2. *Assume the following.*

(i) The potentials $V : \mathbb{R}^3 \to \mathbb{R}$ and $W : \mathbb{R}^3 \to \mathbb{R}$ are spherically symmetric and satisfy $V^2 \lesssim (\mathbb{1} - \Delta)$ and $W^2 \lesssim (\mathbb{1} - \Delta)$ in the sense of forms of operators on $L^2(\mathbb{R}^3)$.

(ii) The normalized one-body spinor

$$\phi \;=\; \begin{pmatrix} u \\ v \\ w \end{pmatrix}\,, \qquad \|\phi\|_{\mathfrak{h}} \;=\; 1$$

is given for some $u,v,w \in H^1(\mathbb{R}^3)$.

(iii) The initial many-body vector state $\psi_N \in \mathcal{H}_N^{\mathrm{s}}$ satisfies $\|\psi_N\|_{\mathcal{H}_N^{\mathrm{s}}} = 1$ and exhibits complete spinor BEC onto ϕ in the quantitative sense

$$\alpha_{(\psi_N,\phi)} \;:=\; 1-\langle\phi,\gamma^{(1)}_{\psi_N}\phi\rangle \;\leqslant\; \frac{K}{N}, \tag{5.21}$$

for some $K>0$.

Correspondingly,

- *let $t\mapsto\psi_{N,t}=e^{-\mathrm{i}tH_N}\psi_N$ be the solution to the Cauchy problem* (5.5) *with the initial datum ψ_N and with the many-body Hamiltonian H_N^{s} defined in* (5.17) *through the potentials V and W fixed by assumption (i);*
- *let $t\mapsto\phi_t=\begin{pmatrix}u_t\\ v_t\\ w_t\end{pmatrix}$ be the solution, with values in $H^1(\mathbb{R}^3)\otimes\mathbb{C}^3$, to the Cauchy problem consisting of the system* (5.20) *with the potentials W and V given by assumption (i) and with the initial datum ϕ.*

Then, for every $t>0$, one has

$$\alpha_{(\psi_{N,t},\phi_t)} \;=\; 1-\langle\phi_t,\gamma^{(1)}_{\psi_{N,t}}\phi_t\rangle \;\leqslant\; \frac{K+1}{N}\,e^{\,Ct} \tag{5.22}$$

and hence also

$$\mathrm{Tr}\left|\gamma^{(1)}_{N,t}-|\phi_t\rangle\langle\phi_t|\right| \;\lesssim\; \frac{1}{\sqrt{N}}\,e^{\,Ct/2} \tag{5.23}$$

for some constant $C>0$ that depends only on W, V, and ϕ.

The proof of Theorem 5.2 can be found in [65], together with a result analogous to Theorem 5.2 for the Gross-Pitaevskii regime.

5.2 Quantitative estimate of the fidelity of the mean-field model

This Section is based on my work [65]. We present a quantitative analysis, based on recent experimental data, of the fidelity of the mean-field regime for the control of condensation. We do it for the spinor BEC model of Section 5.1, by explicitly estimating (5.22) of Theorem 5.2. However, due to the non-restrictive nature of our arguments, the conclusions clearly apply as well for more general systems, including single- and multi-component BEC and pseudo-spinors.

Our main conclusion is going to be that, despite the character of 'first approximation only' of the mean-field model, Theorem 5.2 provides a control of the time-dependent indicator of condensation $\alpha_{(\psi^{\mathrm{phys}}_{N_{\mathrm{exp}},t},\phi^{\mathrm{phys}}_t)}$ that, *for all the typical duration of an experiment on the dynamics of spinor condensates*, remains very small, of the order of the percent (or smaller).

In order to obtain quantitative estimates, we need to briefly revisit the setting presented in Section 5.1 for spinor condensates.

First we restore the physical constants $\hbar$ (Planck's constant) and m (the mass of each bosonic atom), and we take $N = N_{\mathrm{exp}}$, the actual number of particles in a typical experiment. The many-body Hamiltonian (5.17) takes the 'physical' form

$$\begin{aligned} H_{N_{\mathrm{exp}}}^{\mathrm{phys}} \;:=\; & \sum_{j=1}^{N_{\mathrm{exp}}}(-\frac{\hbar^2}{2m}\Delta_{x_j}) + \frac{1}{N_{\mathrm{exp}}}\sum_{1<j\leqslant k<N_{\mathrm{exp}}} W(x_j-x_k) \\ & + \frac{1}{N_{\mathrm{exp}}}\sum_{1<j\leqslant k<N_{\mathrm{exp}}} V(x_j-x_k)\,\boldsymbol{\sigma}_j\bullet\boldsymbol{\sigma}_k\,, \end{aligned} \tag{5.24}$$

the associated linear Schrödinger equation for the 'physical' many-body state $\psi_{N,t}^{\mathrm{phys}}$ becomes

$$\mathrm{i}\hbar\partial_t\psi_{N,t}^{\mathrm{phys}} \;=\; H_{N_{\mathrm{exp}}}^{\mathrm{phys}}\psi_{N,t}^{\mathrm{phys}}\,,$$

and the effective spinor Hartree system (5.20) for the 'physical' one-body orbital $\phi_t^{\mathrm{phys}} = \begin{pmatrix} u_t^{\mathrm{phys}} \\ v_t^{\mathrm{phys}} \\ w_t^{\mathrm{phys}} \end{pmatrix}$ takes the form

$$\begin{aligned} \mathrm{i}\hbar\partial_t\phi_t^{\mathrm{phys}} \;=\; & -\frac{\hbar^2}{2m}\Delta\phi_t^{\mathrm{phys}} + W*\langle\phi_t^{\mathrm{phys}},\phi_t^{\mathrm{phys}}\rangle_{\mathbb{C}^3}\phi_t^{\mathrm{phys}} \\ & + V*\langle\phi_t^{\mathrm{phys}},\boldsymbol{\sigma}\phi_t^{\mathrm{phys}}\rangle_{\mathbb{C}^3}\bullet\boldsymbol{\sigma}\phi_t^{\mathrm{phys}}\,. \end{aligned} \tag{5.25}$$

Let us stress that (5.24) is *not* a mean-field Hamiltonian: the factor N_{exp}^{-1} appears explicitly because of the present choice of the potentials W and V, that are such that $N_{\mathrm{exp}}^{-1}W$ and $N_{\mathrm{exp}}^{-1}V$ are the physical two-body potentials; then, when $N > N_{\mathrm{exp}}$, (5.17) provides the mean-field re-scaled version of the physical Hamiltonian.

We need to qualify a physically realistic initial state $\psi_{N_{\mathrm{exp}},0}^{\mathrm{phys}}$ and physically realistic potentials W_{phys} and V_{phys}.

The many-body initial state must exhibit complete condensation $\psi_{N_{\mathrm{exp}},0}^{\mathrm{phys}} \sim \big(\phi_0^{\mathrm{phys}}\big)^{\otimes N_{\mathrm{exp}}}$ in the quantitative sense (5.21) for the reduced marginal. To be precise, since by construction $\alpha_{(\psi_{N_{\mathrm{exp}},0}^{\mathrm{phys}},\phi_0^{\mathrm{phys}})}$ expresses the initial *depletion* of the Bose gas (i.e., the fraction of particles that do not participate in the condensation), the constant KN_{exp}^{-1} in the bound (5.21) at $t=0$ must bound from above the experimental value for the depletion. In order to match the typical values of depletion (Table 5.1), we take

$$\alpha_{(\psi_{N_{\mathrm{exp}},0}^{\mathrm{phys}},\phi_0^{\mathrm{phys}})} \;\simeq\; 4\cdot 10^{-3}\,. \tag{5.26}$$

Concerning the potentials W_{phys} and V_{phys}, to a very good approximation it is enough to only consider the former and neglect the latter, since in a typical spinor condensate with ^{87}Rb atoms the scattering length c_2 of V_{phys} is by far dominated by the scattering length c_0 of W_{phys} (Table 5.1). In a crude approximation we model W_{phys} as the soft-sphere potential

$$W_{\mathrm{phys}}(x) \;:=\; \begin{cases} W_0 & |x| \;<\; R \\ 0 & |x| \;\geqslant\; R\,, \end{cases} \tag{5.27}$$

	experimental value	*source*
^{87}Rb atomic mass	$1.42 \cdot 10^{-25}$ Kg	
scattering lengths	$c_0 = 57.1\text{Å}, \quad c_2 = -0.53\text{Å}$	[40]
condensate population	$N_{\mathrm{exp}} = 3 \cdot 10^4 \div 3 \cdot 10^5$	[18], [19]
condensate density (n) and depletion (α_0)	$n = 10^{20}\ \mathrm{m}^{-3}$ $\Rightarrow\ \alpha_0 = 4 \cdot 10^{-3}$	[18], [19], [58]
condensate size	$R = 10^{-4}$ m	[18], [19]
equilibration time	$T \lesssim 0.6\,\mathrm{sec}$	[90], [18], [19]

Table 5.1: Experimental values of relevant quantities in typical modern experiments with the dynamical evolution of spinor condensates.

with a radius R that we take to be of the order of the condensate size (Table 5.1) and a magnitude W_0 fixed by the requirement for W_{phys} to have scattering length c_0. A straightforward calculation based on Table 5.1, taking for concreteness $N_{\mathrm{exp}} \simeq 10^5$, allows to find $W_0 \simeq 1.34 \cdot 10^{-34}$ J, and hence

$$W_0/\hbar \;\simeq\; 1.3 \cdot \mathrm{sec}^{-1}\,. \tag{5.28}$$

With these data at hand, repeating for the model now in physical units the very steps that allow to prove Theorem 5.2, yields

$$\alpha_{(\Psi^{\mathrm{phys}}_{N_{\mathrm{exp}},t},\phi^{\mathrm{phys}}_t)} \;\leqslant\; \big(\alpha_{(\Psi^{\mathrm{phys}}_{N_{\mathrm{exp}},0},\phi^{\mathrm{phys}}_0)} + N_{\mathrm{exp}}^{-1}\big)\cdot e^{10\,t\,W_0/\hbar}\,. \tag{5.29}$$

For N_{exp} taken from Table 5.1, the initial value for α given by (5.26), and $W_0/\hbar$ estimated as in (5.28), we see that formula (5.29) produces a control on the indicator of condensation that for times $t \simeq 100\,\mathrm{msec}$, namely of the same order of the duration time of the experiment, is as accurate as

$$\alpha_{(\Psi^{\mathrm{phys}}_{N,t},\phi^{\mathrm{phys}}_t)} \;\leqslant\; 0.015\,, \tag{5.30}$$

thus less than 2%.

As crude as the above estimate is, it shows that the mean-field scaling produces quite an accurate control of the dynamical persistence of condensation when specialized with the actual experimental values.

5.3 Well-posedness of the singular Hartree equation

This Section is based on my work [68].

We shall present a result of well-posedness of the singular Hartree equation in three space dimensions, a version of the ordinary Hartree equation where a local impurity around the point $X = 0$ is modeled, formally, by $V(x) = \delta(x)$, hence producing an equation of the form

$$\mathrm{i}\partial_t u \;=\; \text{“} -\Delta u + \delta(x)u\text{”} + (w * |u|^2)u\,. \tag{5.31}$$

The precise meaning in which the linear part in the r.h.s. of (5.31) has to be understood is the '*singular Hamiltonian of point interaction*', that is, a singular perturbation of the negative Laplacian $-\Delta$ which, consistently with the interpretation of a local impurity that is so singular as to be supported only at one point, is a self-adjoint extension on $L^2(\mathbb{R}^d)$ of the symmetric operator $-\Delta|_{C_0^\infty(\mathbb{R}^d)}$, and therefore acts precisely as $-\Delta$ on H^2-functions supported away from the origin.

In three dimensions one has the following standard construction, which we recall, for example, from [3, Chapter I.1] and [69, Section 3].

The class of self-adjoint extensions in $L^2(\mathbb{R}^3)$ of the positive and densely defined symmetric operator $-\Delta|_{C_0^\infty(\mathbb{R}^3\setminus\{0\})}$ is a one-parameter family of operators $-\Delta_\alpha$, $\alpha \in (-\infty, +\infty]$, defined by

$$\begin{aligned} \mathcal{D}(-\Delta_\alpha) \;&=\; \Big\{\psi \in L^2(\mathbb{R}^3)\,\Big|\, \psi = \phi_\lambda + \frac{\phi_\lambda(0)}{\alpha + \frac{\sqrt{\lambda}}{4\pi}}\, G_\lambda \text{ with } \phi_\lambda \in H^2(\mathbb{R}^3)\Big\} \\ (-\Delta_\alpha + \lambda)\,\psi \;&=\; (-\Delta + \lambda)\,\phi_\lambda\,, \end{aligned} \tag{5.32}$$

where $\lambda > 0$ is an arbitrarily fixed constant and

$$G_\lambda(x) \;:=\; \frac{e^{-\sqrt{\lambda}\,|x|}}{4\pi|x|} \tag{5.33}$$

is the Green function for the Laplacian, that is, the distributional solution to $(-\Delta + \lambda)G_\lambda = \delta$ in $\mathcal{D}'(\mathbb{R}^3)$.

The quadratic form of $-\Delta_\alpha$ is given by

$$\begin{aligned} \mathcal{D}[-\Delta_\alpha] \;&=\; H^1(\mathbb{R}^3) \dotplus \mathrm{span}\{G_\lambda\} \\ (-\Delta_\alpha)[\phi_\lambda + \kappa_\lambda\, G_\lambda] \;&=\; -\lambda\|\phi + \kappa_\lambda\, G_\lambda\|_2^2 \\ &\qquad + \|\nabla\phi\|_2^2 + \lambda\|\phi\|_2^2 + \big(\alpha + \tfrac{\sqrt{\lambda}}{4\pi}\big)\,|\kappa_\lambda|^2\,. \end{aligned} \tag{5.34}$$

The above decompositions of a generic $\psi \in \mathcal{D}(-\Delta_\alpha)$ or $\psi \in \mathcal{D}[-\Delta_\alpha]$ are unique and are valid for every chosen λ. The extension $-\Delta_{\alpha=\infty}$ is the Friedrichs extension and is precisely the self-adjoint $-\Delta$ on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$.

The operator $-\Delta_\alpha$ is reduced with respect to the canonical decomposition

$$L^2(\mathbb{R}^3) \;\cong\; L^2_{\ell=0}(\mathbb{R}^3) \oplus \bigoplus_{\ell=1}^{\infty} L^2_\ell(\mathbb{R}^3)$$

in terms of subspaces $L^2_\ell(\mathbb{R}^3)$ of definite angular symmetry, and it is a non-trivial modification of the negative Laplacian in the spherically symmetric sector only, i.e.,

$$(-\Delta_\alpha)|_{\mathcal{D}(-\Delta_\alpha)\cap L^2_\ell(\mathbb{R}^3)} \;=\; (-\Delta)|_{H^2_\ell(\mathbb{R}^3)}\,, \qquad \ell \neq 0\,. \tag{5.35}$$

Each $\psi \in \mathcal{D}(-\Delta_\alpha)$ satisfies the short range asymptotics

$$\psi(x) \;=\; c_\psi\Big(\frac{1}{|x|} - \frac{1}{a}\Big) + o(1) \qquad \text{as } x \to 0\,, \qquad a := (-4\pi\alpha)^{-1}\,, \tag{5.36}$$

or also, in momentum space,

$$\int_{\substack{p\in\mathbb{R}^3\\|p|<R}} \widehat{\psi}(p)\,\mathrm{d}p \;=\; d_\psi(R+2\pi^2\alpha)+o(1) \qquad \text{as} \qquad R\to+\infty\,, \tag{5.37}$$

for some $c_\psi, d_\psi \in \mathbb{C}$. Equations (5.36) and (5.37) are referred to as, respectively, the *Bethe-Peierls contact condition* [10] and the *Ter-Martyrosyan–Skornyakov condition* [89], and express a boundary condition for the wave function in the vicinity of the origin, which is indeed the characteristic behavior of the low-energy bound state for a Schrödinger operator $-\Delta+V$ where V has almost zero support and s-wave scattering length $a=-(4\pi\alpha)^{-1}$. Thus, $-\Delta_\alpha$ is recognized to be the *Hamiltonian of point interaction in the s-wave channel, localized at $x=0$, and with inverse scattering length α* in suitable units.

The spectrum of $-\Delta_\alpha$ is given by

$$\begin{aligned}\sigma_{\mathrm{ess}}(-\Delta_\alpha) \;&=\; \sigma_{\mathrm{ac}}(-\Delta_\alpha) \;=\; [0,+\infty)\,, \qquad \sigma_{\mathrm{sc}}(-\Delta_\alpha) \;=\; \emptyset\,,\\ \sigma_{\mathrm{p}}(-\Delta_\alpha) \;&=\; \begin{cases} \emptyset & \text{if } \alpha\in[0,+\infty] \\ \{-(4\pi\alpha)^2\} & \text{if } \alpha\in(-\infty,0)\,. \end{cases}\end{aligned} \tag{5.38}$$

The negative eigenvalue $-(4\pi\alpha)^2$, when it exists, is simple and the corresponding eigenfunction is $|x|^{-1}e^{-4\pi|\alpha|\,|x|}$. Thus, $\alpha\geqslant 0$ corresponds to a non-confining, 'repulsive' contact interaction.

We can now make (5.31) unambiguous and therefore consider the singular Hartree equation

$$\mathrm{i}\partial_t u \;=\; -\Delta_\alpha u + (w*|u|^2)u\,. \tag{5.39}$$

In order to avoid non-essential additional discussions, we restrict ourselves once and for all to positive α's. In fact, $-\Delta_\alpha$ is semi-bounded from below for every $\alpha\in(-\infty,+\infty]$, as seen in (5.38) above, thus shifting it up by a suitable constant one ends up with studying a modification of (5.39) with a trivial linear term that does not affect the solution theory of the equation.

Owing to the self-adjointness of $-\Delta_\alpha$, and to its positivity for $\alpha\geqslant 0$, the '*singular (or perturbed) Schrödinger propagator*' $t\mapsto e^{\mathrm{i}t\Delta_\alpha}$ leaves the domain of each power of $-\Delta_\alpha$ invariant. In complete analogy to the non-perturbed case, where the free Schrödinger propagator $t\mapsto e^{\mathrm{i}t\Delta}$ leaves the Sobolev space $H^s(\mathbb{R}^3)=\mathcal{D}((-\Delta)^{s/2})$ invariant, and the solution theory for the ordinary Hartree equation is made in $H^s(\mathbb{R}^3)$, including the energy space $H^1(\mathbb{R}^3)$, now the meaningful spaces of solutions where to settle the Cauchy problem for (5.39) are of the type $\widetilde{H}^s_\alpha(\mathbb{R}^3)$, the '*singular Sobolev space*' of order s, namely the Hilbert space

$$\widetilde{H}^s_\alpha(\mathbb{R}^3) \;:=\; \mathcal{D}((-\Delta_\alpha)^{s/2}) \tag{5.40}$$

equipped with the 'fractional singular Sobolev norm'

$$\|\psi\|_{\widetilde{H}^s_\alpha} \;:=\; \|(\mathbb{1}-\Delta_\alpha)^{s/2}\psi\|_2\,. \tag{5.41}$$

It is worth remarking that whereas the kernel of the propagator $t\mapsto e^{\mathrm{i}t\Delta_\alpha}$ is known since long [87], [2], the characterization of the singular fractional Sobolev space $\widetilde{H}^s_\alpha(\mathbb{R}^3)$ is only a recent achievement [33].

In view of the preceding discussion, we consider the Cauchy problem

$$\begin{cases} \mathrm{i}\partial_t u \;=\; -\Delta_\alpha u + (w*|u|^2)u \\ u(0) \;=\; f \;\in\; \widetilde{H}^s_\alpha(\mathbb{R}^3)\,. \end{cases} \tag{5.42}$$

We are going to discuss its *local* solution theory both in a regime of low (i.e., $s \in [0, \frac{1}{2})$), intermediate (i.e., $s \in (\frac{1}{2}, \frac{3}{2})$), and high (i.e., $s \in (\frac{2}{2}, 2]$) regularity. Then, exploiting the conservation of the mass and of the energy, we are going to obtain a *global* theory in the mass space ($s = 0$) and the energy space ($s = 1$).

We deal with strong $\widetilde{H}^s_\alpha$-solutions of the problem (5.42), meaning, functions $u \in \mathcal{C}(I, \widetilde{H}^s_\alpha(\mathbb{R}^3))$ for some interval $I \subseteq \mathbb{R}$ with $I \ni 0$, which are fixed points for the *solution map*

$$\Phi(u)(t) \;:=\; e^{\mathrm{i}t\Delta_\alpha} f - \mathrm{i}\int_0^t e^{\mathrm{i}(t-\tau)\Delta_\alpha}(w * |u(\tau)|^2)u(\tau)\,\mathrm{d}\tau\,. \tag{5.43}$$

Let us recall the notion of *local* and *global well-posedness* (see [17, Section 3.1]).

Definition 5.3. We say that the Cauchy problem (5.42) is locally well-posed in $\widetilde{H}^s_\alpha(\mathbb{R}^3)$ if the following properties hold:

(i) For every $f \in \widetilde{H}^s_\alpha(\mathbb{R}^3)$, there exists a unique strong $\widetilde{H}^s_\alpha$-solution u to the equation

$$u(t) \;=\; e^{\mathrm{i}t\Delta_\alpha} f - \mathrm{i}\int_0^t e^{\mathrm{i}(t-\tau)\Delta_\alpha}(w * |u(\tau)|^2)u(\tau)\,\mathrm{d}\tau \tag{5.44}$$

defined on the maximal interval $(-T_*, T^*)$, where $T_*, T^* \in (0, +\infty]$ depend on f only.

(ii) There is the blow-up alternative: if $T^* < +\infty$ (resp., if $T_* < +\infty$), then $\lim_{t\uparrow T^*} \|u(t)\|_{\widetilde{H}^s_\alpha} = +\infty$ (resp., $\lim_{t\downarrow T_*} \|u(t)\|_{\widetilde{H}^s_\alpha} = +\infty$).

(iii) There is continuous dependence on the initial data: if $f_n \xrightarrow{n\to+\infty} f$ in $\widetilde{H}^s_\alpha(\mathbb{R}^3)$, and if $I \subset (-T_*, T^*)$ is a closed interval, then the maximal solution u_n to (5.42) with initial datum f_n is defined on I for n large enough, and satisfies $u_n \xrightarrow{n\to+\infty} u$ in $\mathcal{C}(I, \widetilde{H}^s_\alpha(\mathbb{R}^3))$.

If $T_* = T^* = +\infty$, we say that the solution is global. If (5.42) is locally well-posed and for every $f \in \widetilde{H}^s_\alpha(\mathbb{R}^3)$ the solution is global, we say that (5.42) is globally well-posed in $\widetilde{H}^s_\alpha(\mathbb{R}^3)$.

Let us emphasize the following feature of solutions to (5.44): if both f and w are spherically symmetric, so too is u. This follows at once from the symmetry of the non-linear term of (5.44) together with the previously mentioned fundamental property that the subspaces of $L^2(\mathbb{R}^3)$ of definite rotational symmetry are invariant under the propagator $e^{\mathrm{i}t\Delta_\alpha}$. This makes the above definitions of strong solutions and well-posedness meaningful also with respect to the spaces

$$\widetilde{H}^s_{\alpha,\mathrm{rad}}(\mathbb{R}^3) \;:=\; \widetilde{H}^s_\alpha(\mathbb{R}^3) \cap L^2_{\ell=0}(\mathbb{R}^3)$$

equipped with the $\widetilde{H}^s_\alpha$-norm. Part of the solution theory we find is set in such spaces.

We can finally formulate the main results. Let us start with the local theory.

Theorem 5.4 (L^2-theory – local well-posedness)**.** *Let $\alpha \geqslant 0$. Let $w \in L^{\frac{3}{\gamma},\infty}(\mathbb{R}^3)$ for $\gamma \in [0, \frac{3}{2})$. Then the Cauchy problem (5.42) is locally well-posed in $L^2(\mathbb{R}^3)$.*

Theorem 5.5 (Low regularity – local well-posedness)**.** *Let $\alpha \geqslant 0$ and $s \in (0, \frac{1}{2})$. Let $w \in L^{\frac{3}{\gamma},\infty}(\mathbb{R}^3)$ for $\gamma \in [0, 2s]$. Then the Cauchy problem (5.42) is locally well-posed in $\widetilde{H}^s_\alpha(\mathbb{R}^3)$, which in this regime coincides with $H^s(\mathbb{R}^3)$.*

Theorem 5.6 (Intermediate regularity – local well-posedness)**.** *Let $\alpha \geqslant 0$ and $s \in (\frac{1}{2}, \frac{3}{2})$. Let $w \in W^{s,p}(\mathbb{R}^3)$ for $p \in (2, +\infty)$. Then the Cauchy problem* (5.42) *is locally well-posed in $\widetilde{H}^s_\alpha(\mathbb{R}^3)$.*

Theorem 5.7 (High regularity – local well-posedness)**.** *Let $\alpha \geqslant 0$ and $s \in (\frac{3}{2}, 2]$. Let $w \in W^{s,p}(\mathbb{R}^3)$ for $p \in (2, +\infty)$ and spherically symmetric. Then the Cauchy problem* (5.42) *is locally well-posed in $\widetilde{H}^s_{\alpha,\mathrm{rad}}(\mathbb{R}^3)$.*

The transition cases $s = \frac{1}{2}$ and $s = \frac{3}{2}$ are not covered explicitly for the mere reason that the structure of the perturbed Sobolev spaces $\widetilde{H}^{1/2}_\alpha(\mathbb{R}^3)$ and $\widetilde{H}^{3/2}_\alpha(\mathbb{R}^3)$ is not as clean as that of $\widetilde{H}^s_\alpha(\mathbb{R}^3)$ when $s \notin \{\frac{1}{2}, \frac{3}{2}\}$ (see[33]).

Let us remark that for $s > 0$ we have an actual 'continuity' in s of the assumption on w in the three Theorems 5.5, 5.6, and 5.7 above – in the low regularity case our proof does not require any control on derivatives of w and therefore we find it more informative to formulate the assumption in terms of the Lorenz space corresponding to $W^{s,p}(\mathbb{R}^3)$.

Such a 'continuity' is due to the fact that under the hypotheses of Theorems 5.5, 5.6, and 5.7 we can work in a locally-Lipschitz regime of the non-linearity. When instead $s = 0$ we have a 'jump' in the form of an extra range of admissible potentials w, which is due to the fact that for the L^2-theory we are able to make use of the Strichartz estimates for the singular Laplacian.

Next, we investigate the global theory in the mass and in the energy spaces.

Theorem 5.8 (Global solution theory in the mass space)**.** *Let $\alpha \geqslant 0$, and let $w \in L^\infty(\mathbb{R}^3) \cap W^{1,3}(\mathbb{R}^3)$, or $w \in L^{\frac{3}{\gamma},\infty}(\mathbb{R}^3)$ for $\gamma \in (0, \frac{3}{2})$. Then the Cauchy problem* (5.42) *is globally well-posed in $L^2(\mathbb{R}^3)$.*

Theorem 5.9 (Global solution theory in the energy space)**.** *Let $\alpha \geqslant 0$, $w \in W^{1,p}_{\mathrm{rad}}(\mathbb{R}^3)$ for $p \in (2, +\infty)$, and $f \in \widetilde{H}^1_{\alpha,\mathrm{rad}}(\mathbb{R}^3)$.*

(i) There exists a constant $C_w > 0$, depending only on $\|w\|_{W^{1,p}}$, such that if $\|f\|_{L^2} \leqslant C_w$, then the unique strong solution in $\widetilde{H}^1_{\alpha,\mathrm{rad}}(\mathbb{R}^3)$ to (5.42) *with initial data f is global.*

(ii) If $w \geqslant 0$, then the Cauchy problem (5.42) *is globally well-posed in $\widetilde{H}^1_{\alpha,\mathrm{rad}}(\mathbb{R}^3)$.*

As stated in the Theorems above, part of the local and of the global solution theory is set for spherically symmetric potentials w and solutions u. In a sense, this is the natural solution theory for the singular Hartree equation, for sufficiently high regularity. In particular, the spherical symmetry needed for the high regularity theory is induced naturally by the special structure of the space $\widetilde{H}^s_\alpha(\mathbb{R}^3)$ (as opposite to $H^s(\mathbb{R}^3)$, or also to $\widetilde{H}^s_\alpha(\mathbb{R}^3)$ for small s), where a boundary ('contact') condition holds between regular and singular component of $\widetilde{H}^s_\alpha$-functions.

5.4 Derivation of the Gross-Pitaevskii equation with magnetic Laplacian

This Section is based on my work [78]. It contains the non trivial adaptations of the known Pickl's technique [82] which allow to prove the derivation of the time-dependent magnetic Gross-Pitaevskii equation from the many-body dynamics of a dilute gas of identical bosons subject to an external magnetic field.

Given a magnetic vector potential $\mathbf{A} : \mathbb{R}^3 \to \mathbb{R}^3$, the corresponding magnetic Laplacian is defined as

$$-\Delta_{\mathbf{A}} := -(\nabla - \mathrm{i}\mathbf{A})^2.$$

In analogy with the ordinary Sobolev spaces, one defines the magnetic Sobolev space $H^k_{\mathbf{A}}$ as the set of $u \in L^2$ such that

$$\|u\|^2_{H^k_{\mathbf{A}}} = \sum_{0\leqslant j\leqslant k} \|(\nabla - \mathrm{i}\mathbf{A})^j u\|_2^2 < +\infty.$$

We consider, on the Hilbert space $L^2(\mathbb{R}^3)^{\otimes_{\mathrm{sym}} N}$ a many-body Hamiltonian of the form

$$H_N^{\mathrm{mag}} = \sum_{i=1}^N (-\Delta_{\mathbf{A}})_i + \sum_{i<j} N^2 V(N(x_i - x_j)),$$

where the kinetic operator is precisely the magnetic Laplacian, and the pair interaction is rescaled according to the Gross-Pitaevskii regime.

We prove that the effective dynamics of an initially prepared condensate evolving according to H_N^{mag} is ruled by the magnetic Gross-Pitaevskii equation

$$\mathrm{i}\partial_t u_t = -\Delta_{\mathbf{A}} u_t + 8\pi a |u_t|^2 u_t, \tag{5.45}$$

where a is the scattering length of V (see Section 1.3).

The fact that an external magnetic field can be accommodated into the many-body dynamics, and that the one-body marginal can be controlled analogously to what is done when the one-particle operator is simply the negative Laplacian, is to be expected and indeed is mentioned explicitly in [82, Remark 2.1]. However, such an adaptation is not as straightforward as the analogous insertion of an external trapping potential: the magnetic Laplacian is formally the sum of the ordinary Laplacian plus a derivative term that is linear in the magnetic potential and a further quadratic term in the magnetic potential itself; this more complicated structure requires an a priori not immediate adjustment of a number of crucial estimates and steps in the main proof. For the related problem of derivation of the magnetic Hartree equation from many-body quantum dynamics, the reader should refer to [59].

Since we are working in the Gross-Pitaevskii regime, as for Theorem 4.7 and Theorem 5.1, it is important to select a class of initially prepared condensates with an energy compatibility between the many-body and the effective description. To this end, we define the magnetic Gross-Pitaevskii functional

$$\mathcal{E}^{\mathrm{GP,mag}}[u] \;:=\; \int_{\mathbb{R}^3} \big|\big(-\mathrm{i}\nabla + \mathbf{A}(x)\big)u(x)\big|^2 \,\mathrm{d}x + 4\pi a \int_{\mathbb{R}^3} |u(x)|^4 \,\mathrm{d}x. \tag{5.46}$$

We are now ready to state the result.

Theorem 5.10. *Let $V \in L^\infty(\mathbb{R}^3)$ be positive, spherically symmetric, and compactly supported, and let $\mathbf{A} \in W^{1,\infty}(\mathbb{R}^3, \mathbb{R}^3)$ be chosen such that $\nabla \cdot \mathbf{A} = 0$. Consider an initial many-body state $\psi_N \in L^2(\mathbb{R}^3)^{\otimes_{\mathrm{sym}} N}$ exhibiting Bose-Einstein condensation onto some $u \in H^2_{\mathbf{A}}$, i.e. such that*

$$\lim_{N\to\infty} \gamma^{(1)}_{\psi_N} = |u\rangle\langle u|.$$

Suppose in addition that

$$\lim_{N\to\infty} \frac{\langle \psi_N, H_N^{\mathrm{mag}} \psi_N\rangle}{N} \;=\; \mathcal{E}^{\mathrm{GP,mag}}[u].$$

Then condensation is preserved for all $t > 0$, that is, the evolved wave-function $\psi_{N,t} = e^{-\mathrm{i}tH_N^{\mathrm{mag}}}\psi_N$ satisfies

$$\lim_{N\to\infty} \gamma^{(1)}_{\psi_{N,t}} = |u_t\rangle\langle u_t|$$

for u_t solution of the magnetic Gross-Pitaevskii equation (5.45) *with initial datum u.*

We remark that, due to the hypotheses $\mathbf{A} \in W^{1,\infty}$ and $\nabla \cdot \mathbf{A} = 0$, the global existence of solution to the magnetic Gross-Pitaevskii equation (5.45) in the magnetic Sobolev spaces up to $k = 2$ is granted due to standard arguments.

It would be of great interest to find a larger class of vector potentials such that a result similar to Theorem 5.10 holds: for example, a constant magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ is not attainable by $\mathbf{A} \in W^{1,\infty}$. Another interesting future outlook is the derivation of the magnetic Gross-Pitaevskii equation for time-dependent magnetic potentials $\mathbf{A}(t)$. Since the treatment in [82] already deals with time-dependent external (electric) fields, it is expected that such result could be extended to cover a suitable class of $\mathbf{A}(t)$ having enough space and time regularity.

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